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Analysis of Subgrid-Scale Models for Large Eddy Simulation in Turbulent Channel Flow

A bachelor thesis in Applied Mathematics

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Abstract

The problem with simulating turbulent channel flow lies with the computational expense of the small scale effects. To avoid having to calculate such small scales, large eddy simulation is used. Such that the subgrid-scale motions are modelled. Traditional subgrid-scale models do not show perfect agreement with the log-law. This mismatch is analysed and furthermore an adaptive model by Wu and Meyers is derived and applied. The performance of this adaptive model is then compared to traditional models. Finally discretisation errors are discussed which leave room for further improvement.

Contents

1 Introduction

Turbulent flows can be seen all around us, the smoke from a cigarette, the flow over a golf ball or the wind mixing warm and cold air are all examples of turbulent flows. What characterizes a turbulent flow is that it is a chaotic flow. Even though there are deterministic equations which describe turbulent flow, minor changes in initial conditions can lead to dramatic changes in the evolution of the flow.

Figure 1.1: Cigarette smoke starts as a laminar flow, but quickly transitions into turbulent flow.

First attempts to solve fluid flows were made in the 1930s. Obviously no computers were available back then to solve the Navier-Stokes equations, hence the equations were simplified. Often with the use of linearised potential equations or using conformal transformations on 2D flows. However with the increase in computing power, so came the increase in the capability to solving 3D flows. The first attempts to this were made in the late 1960s. Hence computational fluid dynamics is a relatively young branch of mathematics.

An important parameter is the *Reynolds number*. The definition follows from dimension analysis, and is given by

$$\mathrm{Re} \equiv \frac{UL}{\nu}$$

Where U and L are the characteristic velocity- and length scale corresponding to the flow, ν is the kinematic viscosity of the fluid. It represents the ratio of inertial forces to viscous forces. Throughout this report, a Reynolds number of 22600 is considered.

The most obvious way to solve a 3D flow is to directly numerically simulate the flow using the Navier-Stokes equations (DNS). However even for moderate Reynolds numbers (much lower than those in engineering applications) the computational cost is way too high. This is due to the wide range of scales involved in solving turbulent flows. It turns out that the ratio between the largest and smallest scales is proportional to $\mathrm{Re}^{3/4}$ [5]. From this it follows that the number of grid points in three dimensions is proportional to $\mathrm{Re}^{9/4}$. Hence for Reynolds numbers related to real world examples, which are $\mathcal{O}(10^6 - 10^8)$, DNS is too expensive. Since DNS is not applicable in real world situations, models are going to be introduced. However, DNS is not useless, it can be used as a method of verifying the correctness of a model. Often models are tested at (relatively) low Reynolds numbers, such that they can be compared to DNS results.

Another important concept is a so called *eddy*. Eddies are often recognised as vortices, they are parts of the fluid which do not move along with the (mean) flow. The production of eddies is typical for a turbulent flow. Eddies can be produced by *shear stress*, that is, stress caused by passing along a solid boundary. Furthermore these (relatively) large eddies will eventually break down into smaller eddies. Eventually these smaller eddies dissipate due to viscosity. Lewis F.

Richardson, a mathematician and poet, summarised this so called *energy cascade* in the following famous poem

Big whorls have little whorls
That feed on their velocity,
And little whorls have lesser whorls
And so on to viscosity.

An important test case for analysing the performance of models applied in the simulation of flows is *turbulent channel flow*. Often fully developed channel flow is considered, since then the flow is stationary. A more precise description of channel flow will be given in Section 2.

In this report tools of analysing channel flow will be introduced. As well as introducing the mathematical concept of *Large Eddy Simulation* in Section 3. Furthermore several models will be introduced that go along with LES. Some issues with traditional models will be discussed. Finally in Section 5 a new model proposed by Wu and Meyers will be derived, modified and applied.

A three dimensional coordinate system is considered, with coordinate axes in the x, y and z direction (sometimes referred to as x_1, x_2 and x_3 respectively). Corresponding to those directions are the velocity components u, v and w (u_1, u_2 and u_3 respectively). The reader is assumed to have basic knowledge regarding fluid dynamics. Hence the Navier-Stokes equations are given

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1.1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = \mathbf{F} - \frac{1}{\rho}(\nabla p) + \nu \nabla^2 \mathbf{u}$$

F is an external force

ρ is the density

ν is the kinematic viscosity

The first equation governs the conservation of mass, the second is often referred to as the momentum equation. A notation often used in fluid dynamics, and in this report as well, is Einstein notation. A brief description is given in Appendix A. Using this notation, the NS equations become

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = F_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

Furthermore, when considering flow over a wall, boundary conditions are imposed. The no-slip condition together with no-permuation leads to the velocity field being zero along any wall. Throughout this report incompressible & stationary flows under no influence of an external force are considered. This means the NS equations simplify to

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1.2}$$

$$u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{1.3}$$

2 Turbulent channel flow

As mentioned before, the main focus of this report will lie on the modelling and simulation of fully developed turbulent channel flow of a stationary and incompressible fluid. The goal of this section is to characterise and analyse channel flow. Ultimately the so called *law of the wall* will be derived, this gives a relation between the mean stream wise flow and the distance from the wall. Since the relation is independent of the Reynolds number, this makes it a very useful tool for analysing models and simulations.

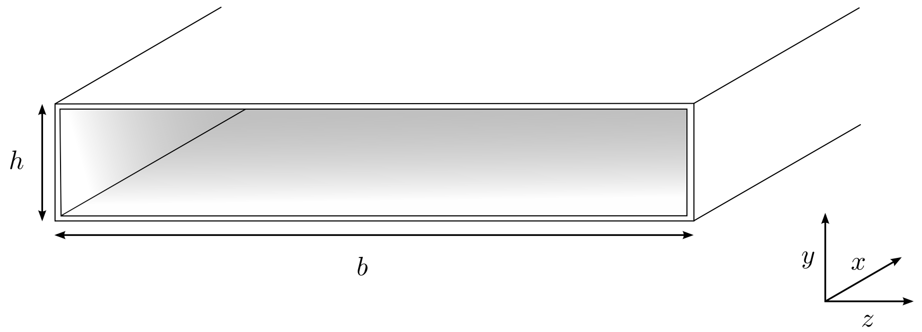


Figure 2.1: Channel flow

A channel flow is a flow through a rectangular duct as illustrated in figure 2.1. Both the length L and the width b of this duct are much bigger than the height $h = 2\delta$. Where δ is the half-height of the duct. Such that

$$\delta \ll L \quad \& \quad \delta \ll b$$

The axes x, y, z are often referred to as:

x: stream wise (or axial)

y: lateral (or wall-normal)

z: span wise

Fully developed channel flow refers to the flow far away from the entrance of the channel, i.e. for large x.

2.1 Flow statistics

Some statistical tools are needed in order to further describe channel flow. The *ensemble average* (mean) of a quantity is denoted by $\langle \cdot \rangle$. The exact definition of $\langle \cdot \rangle$ will be omitted here, however it can be shown that for stationary flow the ensemble average can be replaced by an infinite time averaging operation [10]. This is called the *time ergodicity hypothesis*.

$$\langle f \rangle \equiv \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} f dt$$

This definition also gives rise to the decomposition of f into its mean and fluctuating part

$$f = \langle f \rangle + f'$$

From the definition it is obvious that taking the mean of a quantity commutes with differentiation

$$\left\langle \frac{\partial f(\mathbf{x})}{\partial x_i} \right\rangle = \frac{\partial \langle f(\mathbf{x}) \rangle}{\partial x_i}$$

Also from the linearity of integration it follows that

$$\langle \alpha f + g \rangle = \alpha \langle f \rangle + \langle g \rangle$$

Where α is a constant. Sometimes a quantity of a flow (for example f) is said to be statistically independent of some variable (for example y). Statistical independence means that the mean of that quantity is constant with respect to the variable. So if f is said to be statistically independent of y. This means

$$\frac{\partial \langle f \rangle}{\partial y} = 0$$

2.2 Mean channel flow

Many flow statistics with regard to channel flow are indeed statistically independent. Hence it makes sense to take the mean of the Navier-Stokes equations, since many terms will drop out. To see which quantities are statistically independent consider first the stream wise direction. Since the flow is fully developed, the velocity statistics do not vary with x. Hence

$$\frac{\partial \langle u_i \rangle}{\partial x} = 0$$

Furthermore since $b \gg \delta$, when considering flow away from the walls parallel to the x, y - plane, all flow statistics may be considered independent of z. Also the flow is statistically symmetric about the plane $y = \delta$, this is to be expected but also experimentally confirmed [6]. An important consequence of this is that

$$\langle v \rangle (y) = - \langle v \rangle (h - y) \tag{2.1}$$

The mean flow equations for fully developed channel flow of a stationary incompressible fluid follow from taking the mean $\langle \cdot \rangle$ of Equations (1.1) & (1.3).

Mean continuity

First off the mean continuity equation yields

$$\langle \nabla \mathbf{u} \rangle = \nabla \langle \mathbf{u} \rangle = \frac{\partial \langle u \rangle}{\partial x} + \frac{\partial \langle v \rangle}{\partial y} + \frac{\partial \langle w \rangle}{\partial z} = 0$$

From the previous discussion about statistical independence it follows that $\frac{\partial \langle u \rangle}{\partial x} = \frac{\partial \langle w \rangle}{\partial z} = 0$. And so the continuity equations simplifies to

$$\frac{\partial \langle v \rangle}{\partial y} = 0$$

Since at the boundary $y = 0$ (and $y = 2\delta$) the velocity field is zero, this implies $\langle v \rangle$ is zero everywhere

$$\langle v \rangle = 0$$

Lateral mean momentum

Next consider the lateral mean momentum equation

$$\left\langle u_j \frac{\partial v}{\partial x_j} \right\rangle = -\frac{1}{\rho} \left\langle \frac{\partial p}{\partial y} \right\rangle + \left\langle \nu \frac{\partial^2 v}{\partial x_j \partial x_j} \right\rangle$$

Which can be rewritten by using the continuity equation into

$$\frac{\partial \langle v u_j \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial y} + \nu \frac{\partial^2 \langle v \rangle}{\partial x_j \partial x_j}$$

Since $\langle v \rangle = 0$ and considering that the velocity field varies statistically only in the y direction, this leads to

$$\frac{d\langle v'v' \rangle}{dy} = -\frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial y} \tag{2.2}$$

Integrating Equation (2.2) yields

$$\langle v'v' \rangle + \frac{\langle p \rangle}{\rho} = \langle v'v' \rangle_{y=0} + \frac{\langle p \rangle}{\rho}_{y=0} \tag{2.3}$$

Note that $v_{y=0} = v'_{y=0} = 0$ and define the mean pressure at the wall $y = 0$

$$p_w(x) = \langle p \rangle_{y=o}$$

Note that p_w depends only on x since we consider flow away from the wall parallel to the x, y-plane, such that the flow statistics do not vary with z. Eventually Equation (2.3) becomes

$$\langle v'v' \rangle + \frac{\langle p \rangle}{\rho} = \frac{p_w(x)}{\rho}$$

An important and useful result from this is that

$$\frac{\partial \langle p \rangle}{\partial x} = \frac{dp_w(x)}{dx} \tag{2.4}$$

I.e. the mean stream wise pressure gradient varies only in the stream wise direction.

Stream wise mean momentum

Finally the stream wise mean momentum equation is considered. Taking the mean of the stream wise momentum equation yields

$$\left\langle u_j \frac{\partial u}{\partial x_j} \right\rangle = -\frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x} + \nu \frac{\partial^2 \langle u \rangle}{\partial x_j \partial x_j}$$

Using once again that the velocity field is statistically one-dimensional and Equation (2.4) gives

$$\frac{d\langle uv \rangle}{dy} = -\frac{1}{\rho}\frac{dp_w(x)}{dx} + \nu \frac{d^2\langle u \rangle}{dy^2} \tag{2.5}$$

Moreover since $\langle v \rangle = 0$, Equation (2.5) becomes

$$\frac{d\langle u'v' \rangle}{dy} = -\frac{1}{\rho}\frac{dp_w(x)}{dx} + \nu \frac{d^2\langle u \rangle}{dy^2}$$

Or equivalently

$$\frac{d}{dy}\left[\rho\nu \frac{d\langle u \rangle}{dy} - \rho \langle u'v' \rangle\right] = \frac{dp_w(x)}{dx} \tag{2.6}$$

The quantity between brackets is defined as the *total shear stress* $\tau(y)$

$$\tau(y) \equiv \rho\nu \frac{d\langle u \rangle}{dy} - \rho \langle u'v' \rangle$$

The stress is the sum of the viscous stress $\rho\nu\frac{d\langle u \rangle}{dy}$ and the Reynolds stress $-\rho \langle u'v' \rangle$. The viscous stress is dominant closest to the wall. The Reynolds stress is zero at the boundary (due to the boundary condition) and is dominant away from the wall. Later on specifically how far from the wall which stress is or isn't relevant will be discussed.

Let the *wall shear stress* be defined by

$$\tau_w \equiv \tau(0) = \rho\nu \left(\frac{d\langle u\rangle}{dy}\right)_{y=0} - \underbrace{\rho\langle u'v'\rangle_{y=0}}_{=0 \text{ (Bdy. cond.)}} = \rho\nu\left(\frac{d\langle u\rangle}{dy}\right)_{y=0}$$

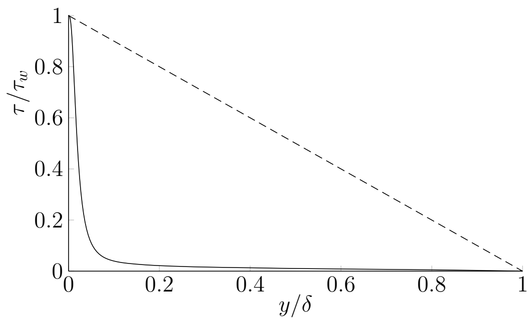
From Equation (2.6) it follows that both $\frac{dp_w(x)}{dx}$ and $\frac{d\tau(y)}{dy}$ are constant (and equal). Hence $\tau(y)$ is a linear function, from this it follows that one more point $(y, \tau(y))$ is needed in order to obtain an equation for $\tau(y)$ in terms of τ_w. Here the symmetry property of the flow is used, from Equation (2.1) it follows that

$$\tau(y) = \tau_w\left(1 - \frac{y}{\delta}\right)$$

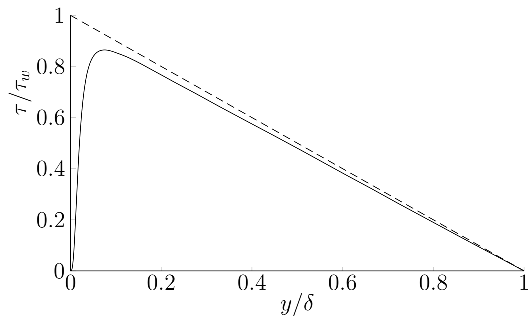
Moreover from Equation (2.6) it follows that

$$\frac{dp_w(x)}{dx} = \frac{d\tau(y)}{dy} = -\frac{\tau_w}{\delta}$$

The contributions of the viscous and Reynolds stress from DNS data are shown in figure 2.2.



(a) Solid: Viscous stress. Dashed: Total stress



(b) Solid: Reynolds stress. Dashed: Total stress

Figure 2.2: Contributions of the viscous shear stress, and the Reynolds shear stress in turbulent channel flow: DNS data of Kim et al. [1].

2.3 Law of the wall

As mentioned before, the main goal of this section is to arrive at the law of the wall. This law will be used later on to judge the performance of several models used to refine LES.

The most important thing to notice from the previous sections is that fully developed channel flow is statistically one dimensional. Furthermore the *only* non-zero velocity statistic is $\langle u\rangle$ and it varies only in the wall-normal direction. From Equation (2.6) it follows that the fully developed flow is entirely determined by $y, \nu, \rho, \frac{dp_w}{dx}$ and of course the channel half-height δ.

Viscous scales

In the near-wall region small length scales are significant, hence viscous scales are introduced. The *friction velocity* is given by

$$u_\tau \equiv \sqrt{\frac{\tau_w}{\rho}}$$

And the *viscous length scale*

$$\delta_\nu \equiv \nu\sqrt{\frac{\rho}{\tau_w}} = \frac{\nu}{u_\tau}$$

Furthermore the friction Reynolds number is

$$\mathrm{Re}_\tau \equiv \frac{u_\tau \delta}{\nu} = \frac{\delta}{\delta_\nu}$$

Alternatively to measuring the distance from the wall in $\frac{y}{\delta}$, it can be measured in the viscous length scale δ_ν

$$y^+ \equiv \frac{y}{\delta_\nu} = \frac{y u_\tau}{\nu}$$

The normalised mean velocity is given by

$$u^+ \equiv \frac{\langle u \rangle}{u_\tau}$$

The definition of y^+ gives rise to several layers within the near wall region:

Wall-normal distance	Layer name	Viscous stress	Reynolds stress
$y^+ < 5$	*Viscous sublayer*	Yes	Negligible
$y^+ < 50$	*Viscous wall region*	Yes	Yes
$y^+ > 50$	*Outer layer*	Negligible	Yes

Table 1: Several near wall regions

Note that this separation of the channel flow into separate layers can be motivated by DNS data presented in figure 2.3.

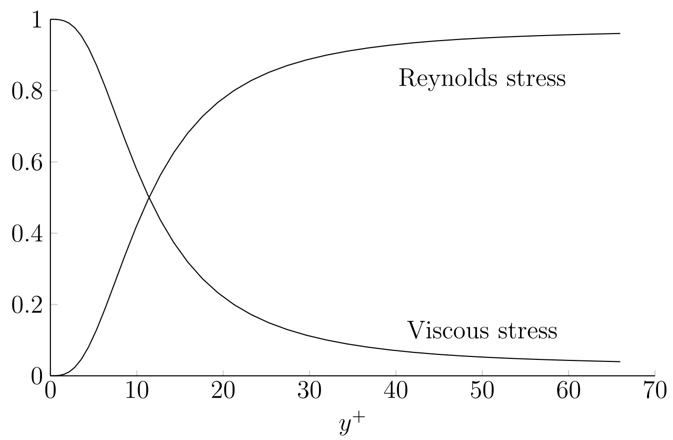


Figure 2.3: Contribution of Reynolds and viscous stress. DNS data of Kim et al. [1].

Furthermore based on the wall-normal distance relative to the channel half-height $\frac{y}{\delta}$, also an *inner layer* may be recognized. This was initially proposed by Prandtl: he stated that (at a high Reynolds number) whenever $\frac{y}{\delta} < 0.1$, the mean velocity would depend only on the viscous scales. Hence being independent of δ and the centreline velocity (the mean velocity along $y = \delta$).

Finally the last length scale which will be introduced is a length scale for the *wall roughness*. Imagine for example a duct with grains of sand stuck to the wall, here the length scale would be the average distance between the grains of sand, hence causing small protrusions in the wall. This length scale is denoted by y_0. Obviously whenever $y_0 \ll \delta_\nu$ this length scale will have no effect on the flow. Whenever this holds, the wall is considered *smooth*. However in some applications the roughness length scale is much larger than the viscous length scale. Here the flow is expected to indeed depend on y_0. Note that in between these two extreme cases, there is the situation where $y_0 \approx \delta_\nu$. This is called a transitionally rough wall. Only smooth walls are considered in this report.

Derivation of the law of the wall

Consider a smooth wall, hence no dependence on y_0. From the viscous scales it follows that the dependence of the flow on $\frac{dp_w}{dx}$ can also be expressed as a dependence on u_τ, since

$$u_\tau \equiv \sqrt{\frac{\tau_w}{\rho}} = \sqrt{-\frac{\delta}{\rho}\frac{dp_w}{dx}}$$

Also the dependence on ν can be replaced by a dependence on δ_ν. From this it follows that the mean stream wise velocity gradient is a function of y, δ_ν, δ and u_τ (the dependence on ρ is omitted since the velocity gradient is implicitly dependent on it via u_τ).

Dimension analysis yields the choice of three dimensionless groups: $\frac{y}{\delta}$, $\frac{y}{\delta_\nu}$ and $\frac{\delta_\nu}{\delta}$. This leads to the following

$$\frac{d\langle u\rangle}{dy} = \frac{u_\tau}{y}\Phi\left(\frac{y}{\delta_\nu}, \frac{y}{\delta}\right) \tag{2.7}$$

Furthermore only the inner-layer is considered, i.e. $\frac{y}{\delta} < 0.1$, so from Prandtls proposal the dependence on δ vanishes. Hence a new function is introduced

$$\Phi_1\left(\frac{y}{\delta_\nu}\right) \equiv \lim_{\frac{y}{\delta}\to 0} \Phi\left(\frac{y}{\delta_\nu}, \frac{y}{\delta}\right) \tag{2.8}$$

It follows from Equation (2.7) & (2.8) that

$$\frac{d\langle u\rangle}{dy} = \frac{u_\tau}{y}\Phi_1\left(\frac{y}{\delta_\nu}\right) \tag{2.9}$$

Integrating Equation (2.9) yields the *law of the wall* for smooth walls

$$u^+ = \int_0^{y^+} \frac{1}{y'}\Phi_1(y')\,dy' \equiv f_w(y^+) \tag{2.10}$$

Viscous sublayer

First the viscous sublayer is considered, hence $y^+ < 5$. The law of the wall then simplifies to (up to third order approximation, see Appendix C)

$$u^+ = f_w(y^+) = y^+$$

Which is confirmed by using DNS data , it shows good agreement for $y^+ < 5$. As can be seen in Figure 2.4

Log-law region

Finally the so called *log-law region* is considered. This region is on the 'outside' of the inner layer. Usually the log-law region is taken to be $y^+ > 30$ and $\frac{y}{\delta} < 0.3$. However it is still assumed that Prandtls hypothesis holds, i.e. no dependence on the large scales.

First consider having a smooth wall, then since $y^+ > 30$, it may be assumed that also the viscous effects are negligible. Hence also the dependence of Φ_1 on δ_ν vanishes. So Φ_1 is constant

$$\Phi_1 = \frac{1}{\kappa} \tag{2.11}$$

Where κ is the *von Kármán* constant. Equation (2.10) now yields

$$u^+ = \int_0^{y^+} \frac{1}{y'}\Phi_1(y')\,dy' = \int_0^{y^+} \frac{1}{\kappa y'}dy' = \frac{1}{\kappa}\ln y^+ + B \tag{2.12}$$

The constants κ and B are generally within 5% of [6]

$$\kappa = 0.41, \qquad B = 5.2$$

Equation (2.12) is called the log-law, it is a relationship between the normalised stream wise mean velocity and the distance from the wall. It is used to judge the performance of wall-models (this will be discussed in section 4.1). Figure 2.4 shows how well the log-law matches DNS data.

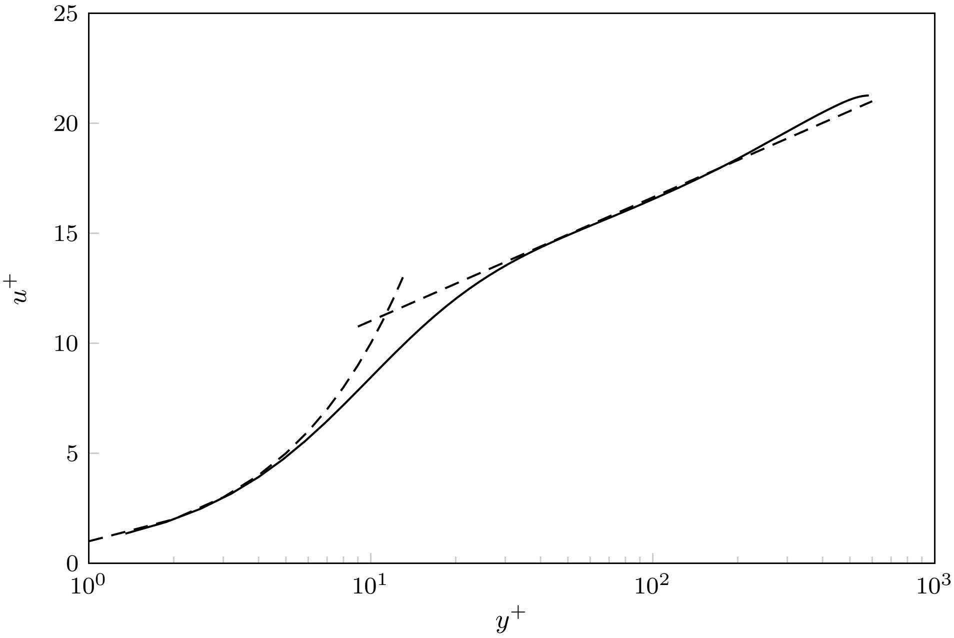


Figure 2.4: Dashed: theoretical law of the wall. Solid: DNS data of Kim et al.

3 Large eddy simulation

As mentioned before DNS has a very high computational cost, which makes it inapplicable in actual engineering situations (Number of grid points is proportional to $\mathrm{Re}^{9/4}$ [5]). Most of this computation time however is spend in calculating the small scale motions of the fluid. To prevent having to fully resolve these small scale motions, LES was introduced. LES stands for Large Eddy Simulation, i.e. the large scale motions of the fluid are resolved, while the small scale motions are modelled. LES is based on separating the velocity field and pressure into large and small scale quantities. This is referred to as filtering. The filtered velocity field consists only of the large scales of motion.

The filtering operation is defined by a filter kernel, this kernel defines in which way the velocity field and pressure are filtered. And hence determines the size of the largest eddies which are still simulated.

3.1 Filters

Intuitively a filter can be seen as an operation on a function which removes 'noise'. In the case of fluid dynamics this noise are the small scale eddies which considered to be too expensive to compute. The velocity field obviously depends on three spatial dimensions, however in this introduction to filters, only one spatial dimension will be considered. In this way, the filtering operation can easily be represented in terms of its frequency damping effect.

Consider a function $f = f(x)$, which will be filtered. The filtered function will be denoted by $\bar{f}$. The definition is as follows

$$\bar{f}(x) \equiv (f * G) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(r,x)f(x-r)dr \tag{3.1}$$

Hence $\bar{f}$ is the convolution of f with the filter kernel G. G is such that the integral over the entire domain of G is 1. Moreover, the filtering operation allows f to be written as the sum of the large-scale part $\bar{f}$ and the small-scale part f^*

$$f = f^* + \bar{f}$$

Note that often f' is used to denote the small scale part, however this notation is used already as the fluctuating part of f after ensemble averaging. As in Section 2.1.

Properties

Some important properties of the filtering operation will be given here. Most of them follow directly from the definition.

1. Linearity
$$\overline{f+g} = \bar{f} + \bar{g}$$
2. Scalar multiplication
$$\overline{\alpha f} = \alpha \bar{f}$$
3. Differentiation commutes. This holds only for homogeneous filters
$$\overline{\frac{\partial f}{\partial x_i}} = \frac{\partial \bar{f}}{\partial x_i}$$
and
$$\overline{\frac{\partial f}{\partial t}} = \frac{\partial \bar{f}}{\partial t}$$
4. Filtering may be interpreted as a projection. Hence the following holds
$$\bar{\bar{f}} = \bar{f}$$
But also
$$\overline{f^*} = 0$$

Proof of the third property can be found in Appendix B.

Common filters

In LES there are three filters which are most commonly used. To give more intuition into the effect of applying such a filter, their Fourier transforms are considered as well. Important to note is the following theorem

Theorem 1.
$$\mathcal{F}(\bar{f}) = \mathcal{F}\{f * G\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{G\}$$

The use of this theorem allows the analysis of each of the filter kernels. It shows that the amplitude is damped by the Fourier transform of the corresponding kernel. The most commonly used filters are the following, they are all homogeneous filters, hence $G(r,x) = G(r)$.

Top-hat filter The top-hat filter, or sometimes called the box filter, simply gives the average value over the interval $(r - \Delta/2, r + \Delta/2)$. The kernel is given by

$$G(r) = \begin{cases} \frac{1}{\Delta} & \text{if } |r| < \frac{\Delta}{2}, \\ 0 & \text{otherwise} \end{cases}$$

Note that this, and all the other kernels considered here, is a homogeneous kernel ($G(r, x) = G(r)$). The Fourier transform of the top-hat kernel is given by

$$\hat{G}(\omega) = \frac{\sin\left(\frac{\omega\Delta}{2}\right)}{\frac{\omega\Delta}{2}}$$

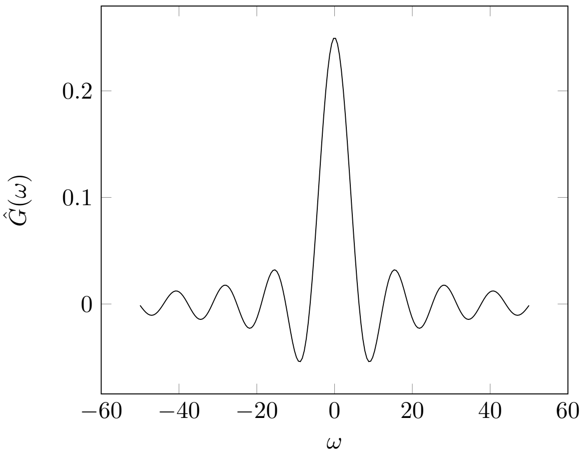


Figure 3.1: Fourier transform of the top-hat filter for $\Delta = 1$

This shows that the top-hat filter smoothly damps high frequencies. For spatially filtering a velocity field this corresponds to damping the small scale motions.

Gaussian filter The kernel of the Gaussian filter is given by

$$G(r) = \sqrt{\frac{6}{\pi\Delta^2}} \exp\left(-\frac{6r^2}{\Delta^2}\right)$$

It's Fourier transform is also a Gaussian curve, and it is given by

$$\hat{G}(\omega) = \exp\left(-\frac{\omega^2\Delta^2}{24}\right)$$

It's amplitude spectrum looks like

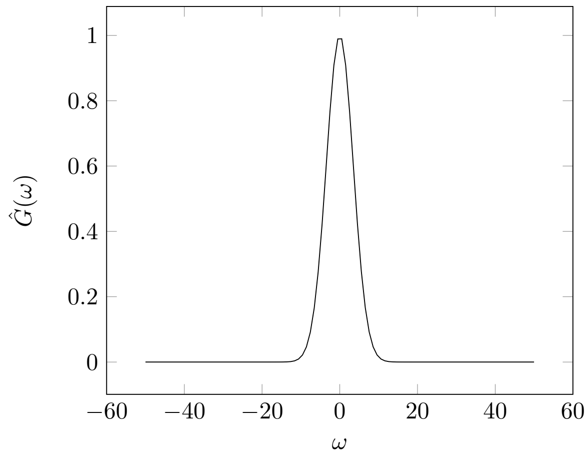


Figure 3.2: Fourier transform of the Gaussian filter for $\Delta = 1$

Sharp spectral filter Finally the sharp spectral filter is considered. This filter simply cuts off the amplitude spectrum at a desired frequency. The kernel is given by

$$G(r) = \frac{\sin\left(\frac{\pi r}{\Delta}\right)}{\pi r}$$

It's Fourier transform is given by

$$\hat{G}(\omega) = \mathrm{rect}_{\frac{2\pi}{\Delta}}(\omega) = \begin{cases} 1 & |\omega| < \frac{\pi}{\Delta}, \\ 0 & |\omega| > \frac{\pi}{\Delta}, \\ \frac{1}{2} & |\omega| = \frac{\pi}{\Delta} \end{cases}$$

Which looks like

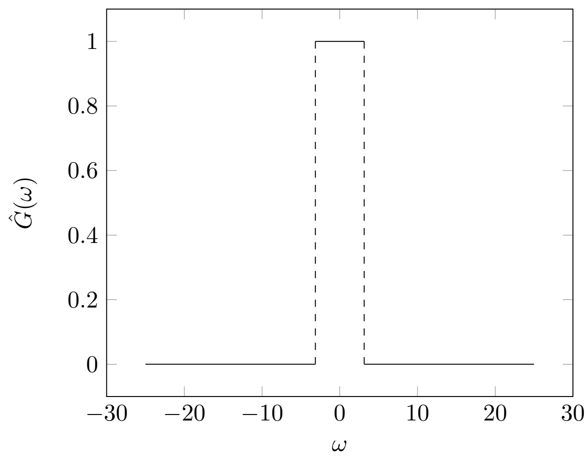


Figure 3.3: Fourier transform of the sharp spectral filter for $\Delta = 1$

The application of such filters on the NS equations (in 3D) is a simple extension of the filters mentioned above. For example the top-hat filter in three spatial dimensions is defined as

$$G(\mathbf{r}) = \begin{cases} \frac{1}{\Delta_1 \Delta_2 \Delta_3} & \text{if } |r_i| < \frac{\Delta_i}{2} \quad (i = 1, 2, 3), \\ 0 & \text{otherwise} \end{cases}$$

3.2 Filtering the Navier-Stokes equations

Now that filters are introduced this concept may be applied to the NS equations, such that the NS equations in terms of the filtered velocity field and pressure are obtained. Recall the NS Equations (1.2) & (1.3). Simply filtering the equations yields (considering no external forces)

$$\overline{\frac{\partial u_j}{\partial x_j}} = 0 \tag{3.2}$$

$$\overline{u_j \frac{\partial u_i}{\partial x_j}} = -\overline{\frac{1}{\rho}\frac{\partial p}{\partial x_i}} + \nu \overline{\frac{\partial^2 u_i}{\partial x_j \partial x_j}} \tag{3.3}$$

A homogeneous filter will be considered such that filtering commutes with taking any spatial or time-derivative, hence the continuity Equation (3.2) simplifies to

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0$$

I.e. the filtered velocity agrees to the continuity equation. As for the momentum equation, using the continuity equation, equation (3.3) can be written as

$$\frac{\partial \overline{u_i u_j}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} \tag{3.4}$$

Unfortunately $\bar{\mathbf{u}}$ does not satisfy the second NS equation due to the presence of the non-linear term $\overline{u_i u_j}$. Directly solving (3.4) would require the full velocity field $\mathbf{u}$ to be resolved, which defeats the purpose of LES. In order to get closer to the form of the momentum equation the *residual-stress tensor* is introduced

$$\tau_{ij}^R \equiv \overline{u_i u_j} - \bar{u}_i \bar{u}_j$$

Moreover it is beneficial to make the residual-stress tensor trace-less by subtracting the so called *isotropic residual stress* from the residual-stress tensor

$$\tau_{ij}^r \equiv \tau_{ij}^R - \frac{1}{3}\tau_{kk}^R \delta_{ij}$$

Where δ_{ij} is the Kronecker delta. τ_{ij}^r is called the *anisotropic-stress tensor*. This gives

$$\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}^r}{\partial x_j} - \frac{1}{3}\frac{\partial \tau_{kk}\delta_{ij}}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} \tag{3.5}$$

Where $-\frac{1}{3}\frac{\partial \tau_{kk}\delta_{ij}}{\partial x_j}$ was added to compensate for introducing the anisotropic-stress tensor. This term simplifies to

$$\frac{1}{3}\frac{\partial \tau_{kk}\delta_{ij}}{\partial x_j} = \frac{1}{3}\frac{\partial \tau_{kk}}{\partial x_i}$$

This term is usually included in the modified filtered pressure

$$\bar{p} \equiv \overline{p} + \frac{1}{3}\rho \tau_{kk}$$

Such that (3.5) becomes

$$\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}^r}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2}$$

Finally the filtered rate-of-strain tensor is introduced as being the symmetric part of $\frac{\partial \bar{u}_i}{\partial x_j}$

$$\bar{S}_{ij} \equiv \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)$$

Which leads to the filtered Navier-Stokes equations

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \tag{3.6}$$

$$\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\nu \bar{S}_{ij} - \tau^r_{ij}\right) \tag{3.7}$$

Simply counting the number of equations and variables included in Equations (3.6) & (3.7) shows that the equations are not *closed*. Several approaches to solving this problem will be introduced in the following sections.

3.3 Eddy-viscosity model

From Equations (3.6) & (3.7) it is clear that a model for the only remaining unfiltered quantity is needed: the anisotropic stress tensor τ^r_{ij}. Modelling this quantity will close the equations, such that they can be solved (numerically).

Such a model is referred to as a *subgrid-scale model* (or SGS model) since often the filter width Δ is chosen equal to the grid size. Hence the sub-grid scale effects are modelled. The most common model was introduced by Smagorinsky in 1963 and is hence called the Smagorinsky model. Many other (more advanced) models are based on this rather simple model by Smagorinsky.

The model is based on the so called Boussinesq hypothesis. Which states that the anisotropic stress tensor is linearly dependent on the filtered rate-of-strain tensor. Such a model is called a *linear eddy-viscosity model.*

$$\tau^r_{ij} = -2\nu_r \bar{S}_{ij} \tag{3.8}$$

The coefficient ν_r is the *eddy viscosity of the residual motions.* Substituting Equation (3.8) into the filtered momentum equation (3.7) yields

$$\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\bar{S}_{ij}\left[\nu + \nu_r\right]\right)$$

Hence the model adds the effect of the small eddies as an addition to the molecular viscosity. There are several approaches to modelling ν_r, however only a few will be mentioned here.

Smagorinsky

Smagorinsky was the first to propose such an eddy-viscosity model, it is called the Smagorinsky-Lilly model

$$\nu_r = l_s^2|\bar{S}| = (C_s\Delta)^2\,|\bar{S}|$$

Where l_s is the *Smagorinsky length scale*, C_s the *Smagorinsky coefficient* and $\bar{S}$ is the characteristic filtered rate-of-strain, which is defined as

$$|\bar{S}| \equiv \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$$

Prandtl

Another model, proposed by Prandtl, involves Prandtl's *mixing length* $l_s = ky$. Such that the model becomes

$$\nu_r = l_s^2|\bar{S}| = (\kappa y)^2\,|\bar{S}|$$

κ is the von Kármán constant.

Mason & Thompson

Finally an algebraic model proposed by Mason & Thompson [2]

$$\frac{1}{l_s} = \frac{1}{C_s\Delta} + \frac{1}{\kappa y}$$

Such that for large y the Smagorinsky length scale reduces to the model proposed by Smagorinsky. This model will be applied later on.

4 Performance of LES

4.1 The log-law

Now the question is: How well does LES perform compared to DNS? LES might be a more efficient method, and more applicable. But if the results do not match those of DNS, the method is rather useless.

Since especially small scale effects are more important near the wall, the inner-layer is considered. Moreover since the Reynolds stress is modelled, in particular the region where this stress is dominant is most interesting. Hence the log-law region is considered, $y^+ > 30$ & $\frac{y}{\delta} < 0.3$. Recall from Section 2.3 that in the log-region the following normalised mean velocity is expected

$$\frac{\langle u \rangle}{u_\tau} = u^+ = \frac{1}{\kappa} \ln y^+ + B$$

It has already been mentioned that indeed this law holds very well for DNS calculations (see figure 2.4). More interesting to see is whether or not the same holds for LES. It turns out that when using traditional Smagorinsky type models the log-law holds only partially. When using the traditional model by Mason & Thompson, the following is obtained:

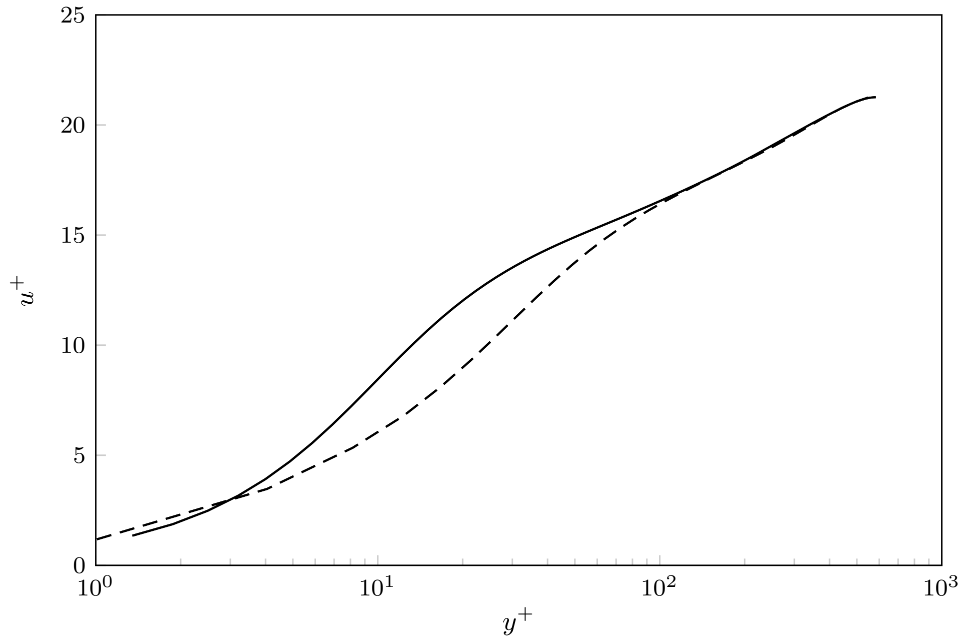


Figure 4.1: Velocity profile. Solid: DNS data of Kim et al. [1]. Dashed: LES data using Mason & Thompson model.

For this model the buffer layer (in-between the viscous sublayer and the outer layer), is large compared to results obtained by DNS. The velocity profile tends to a log profile only around

$y^+ \approx 70$. Another useful way to analyse this observed log-layer mismatch, is to look at the normalised mean velocity gradient. Which is defined by

$$\phi(y) \equiv \frac{y\kappa}{u_\tau}\frac{d\langle u\rangle}{dy}$$

Conveniently, in the log-law region the mean velocity gradient is equal to $\frac{u_\tau}{y\kappa}$ (from Equation (2.11)) such that

$$\phi(y) = 1$$

Indeed when considering DNS the normalised mean velocity gradient is approximately one in the log-law region, see Figure 4.2. Furthermore note that the normalised mean velocity gradient from using LES shows a significant mismatch.

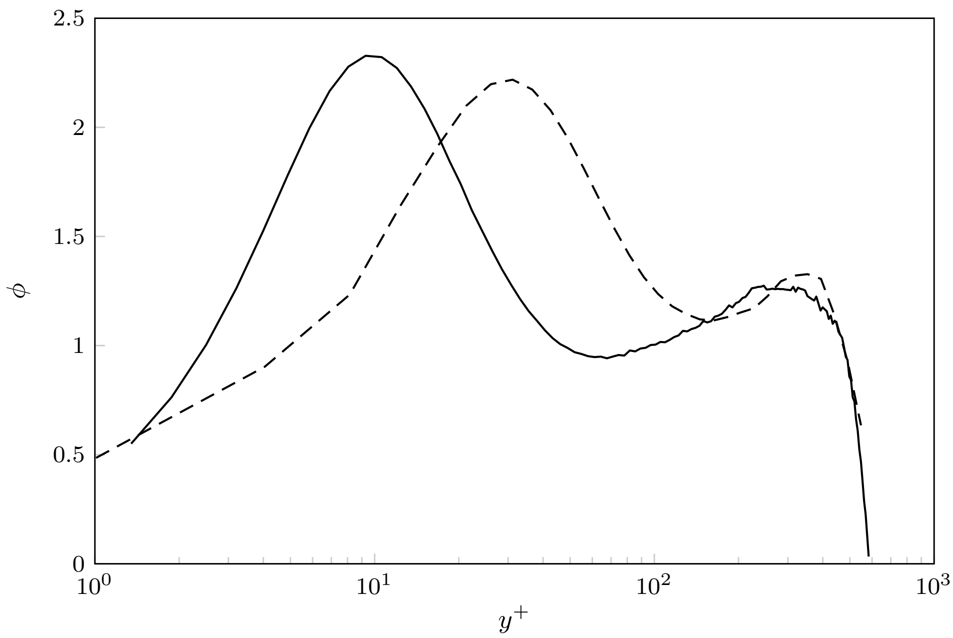


Figure 4.2: Normalised mean velocity gradient. Solid: DNS data of Kim et al. [1]. Dashed: LES using traditional model by Mason & Thompson.

4.2 Analysis of energy contributions

From the previous section it is known that traditional LES models do not behave according to the log-law (hence the normalised mean velocity gradient is not approximately one in the log-law region). So it is interesting to know which energy contributes most to $\phi(y)$, such that the source of the problem can be derived. Before looking at LES however, the energy contributions concerning DNS are considered.

DNS - energy contributions

Recall the mean stream wise momentum equation (2.6)

$$\frac{d}{dy}\left[\nu\frac{d\langle u\rangle}{dy} - \langle u'v'\rangle\right] = -f \tag{4.1}$$

Where

$$f = -\frac{1}{\rho}\frac{dp_w(x)}{dx} = -\frac{1}{\rho}\frac{d\tau(y)}{dy} = \frac{\tau_w}{\rho\delta} \tag{4.2}$$

is the mean pressure gradient. Integration of Equation (4.1) from 0 to y yields

$$\nu\frac{d\langle u\rangle}{dy} - \langle u'v'\rangle - \nu\frac{d\langle u\rangle}{dy}_{y=0} + \langle u'v'\rangle_{y=0} = -f(y-0)$$

Which, using the boundary condition, the definition of u_τ and Equation (4.2) leads to

$$\nu\frac{d\langle u\rangle}{dy} - \langle u'v'\rangle = -fy + u_\tau^2 = f(\delta - y)$$

The usefulness of this relation will be apparent later on. Now consider the turbulent kinetic energy equation (its derivation can be found in Appendix D.1)

$$0 = \underbrace{-\frac{d}{dy}\langle qv'\rangle}_{\text{turb. convection}} \underbrace{-\langle u'v'\rangle\frac{d\langle u\rangle}{dy}}_{\text{production}} \underbrace{-\frac{1}{\rho}\frac{d}{dy}\langle v'p'\rangle}_{\text{pressure trans.}} \underbrace{+\nu\frac{d^2k}{dy^2}}_{\text{viscous diff.}} \underbrace{-\nu\left\langle\frac{\partial u_i'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}\right\rangle}_{\text{pseudo-diss.}}$$

Where $q \equiv \frac{u_i'u_i'}{2}$ and $k \equiv \frac{\langle u_i'u_i'\rangle}{2}$. Furthermore the pseudo-dissipation term can be split in to a turbulent dissipation and viscous diffusion term. The derivation is omitted here and can be found in Appendix D.3.

When adding and subtracting the mean flow viscous dissipation $\nu\left(\frac{d\langle u\rangle}{dy}\right)^2$, the turbulent kinetic energy equation becomes

$$0 = \tilde{P} - \tilde{\epsilon} - T$$

Where $\tilde{P}$ is a modified production term, $\tilde{\epsilon}$ is a dissipation term and T is a transport term. They are defined as follows

$$\begin{aligned}
\tilde{P} &= -\langle u'v'\rangle\frac{d\langle u\rangle}{dy} + \nu\left(\frac{d\langle u\rangle}{dy}\right)^2 \\
\tilde{\epsilon} &= 2\nu\left\langle S_{ij}'S_{ij}'\right\rangle + \nu\left(\frac{d\langle u\rangle}{dy}\right)^2 \\
T &= \frac{d}{dy}\langle qv'\rangle + \frac{1}{\rho}\frac{d}{dy}\langle v'p'\rangle - \nu\frac{d^2k}{dy^2} - \nu\frac{d^2}{dy^2}\langle v'v'\rangle
\end{aligned} \tag{4.3}$$

Equation (4.3) allows the mean velocity gradient to be written as

$$\frac{d\langle u\rangle}{dy} = \frac{\tilde{P}}{-\langle u'v'\rangle + \nu\frac{d\langle u\rangle}{dy}} = \frac{\tilde{P}}{u_\tau^2 - fy}$$

Such that the normalised mean velocity gradient becomes

$$\phi(y) = \frac{y\kappa}{u_\tau(u_\tau^2 - fy)}(\tilde{\epsilon} + T)$$

Hence it is the normalised sum of dissipation and transport terms which come from the turbulent kinetic energy equation.

LES - energy contributions

A similar analysis can be made with the use of the LES turbulent kinetic energy equation. The mean stream wise momentum equation for the filtered velocity field follows from taking the mean of Equation (3.7). Also the flow is considered to be stationary . Hence the stream wise momentum equation becomes (using the statistical one-dimensionality of the channel flow)

$$\frac{d\langle\bar{u}\bar{v}\rangle}{dy} = -\frac{1}{\rho}\frac{d\langle\bar{p}\rangle}{dx} + \nu\frac{d^2\langle\bar{u}\rangle}{dy^2} - \frac{d\langle\tau_{12}^r\rangle}{dy}$$

Since $\langle \bar{v} \rangle = 0$ this simplifies to

$$\frac{d}{dy}\left[-\langle \bar{u}'\bar{v}'\rangle + \nu \frac{d\langle \bar{u}\rangle}{dy} - \langle \tau_{12}^{r}\rangle\right] = -f \tag{4.4}$$

Where $f = -\frac{1}{\rho}\frac{d\langle \bar{p}\rangle}{dx}$. Such that upon integration, Equation (4.4) becomes

$$-\langle \bar{u}'\bar{v}'\rangle + \nu \frac{d\langle \bar{u}\rangle}{dy} - \langle \tau_{12}^{r}\rangle = \frac{\tau_w}{\rho} - fy = u_\tau^2 - fy = f(\delta - y)$$

Note that the wall shear stress is now defined as $\tau_w = \left[-\rho \langle \bar{u}'\bar{v}'\rangle + \rho\nu\frac{d\langle \bar{u}\rangle}{dy} - \rho\langle \tau_{12}^{r}\rangle\right]_{y=0}$. Equivalently to the previous analysis, the turbulent kinetic energy equation is considered. The derivation for this equation for LES can be found in Appendix D.2.

$$0 = -\frac{d}{dy}\langle \bar{q}\bar{v}'\rangle - \langle \bar{u}'\bar{v}'\rangle \frac{d\langle \bar{u}\rangle}{dy} - \frac{1}{\rho}\frac{d}{dy}\langle \bar{v}'\bar{p}'\rangle - \frac{d}{dy}\left\langle \bar{u}_i'\tau_{i2}^{r'}\right\rangle + \left\langle \frac{\partial \bar{u}_i'}{\partial x_j}\tau_{ij}^{r'}\right\rangle + \nu\left\langle \bar{u}_i'\frac{\partial^2 \bar{u}_i'}{\partial x_j \partial x_j}\right\rangle$$

Where $\bar{q} \equiv \frac{\bar{u}_i'\bar{u}_i'}{2}$. Next the mean flow SGS dissipation $\langle \tau_{12}^{r}\rangle \frac{d\langle \bar{u}\rangle}{dy}$ and the mean flow viscous dissipation $\nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2$ are added and subtracted, furthermore the terms are reorganised to obtain

$$0 = \tilde{P}_{\text{LES}} - \tilde{\epsilon}_{\text{LES}} - T_{\text{SGS}} - T_{\text{RES}}$$

The third term is the SGS transport term, and the last term represents the resolved turbulent transport. The terms are given by

$$\begin{aligned}
\tilde{P}_{\text{LES}} &= -\langle \bar{u}'\bar{v}'\rangle \frac{d\langle \bar{u}\rangle}{dy} - \langle \tau_{12}^{r}\rangle \frac{d\langle \bar{u}\rangle}{dy} + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 \\
\tilde{\epsilon}_{\text{LES}} &= -\left\langle \frac{\partial \bar{u}_i'}{\partial x_j}\tau_{ij}^{r'}\right\rangle - \langle \tau_{12}^{r}\rangle \frac{d\langle \bar{u}\rangle}{dy} + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 \\
T_{\text{SGS}} &= \frac{d}{dy}\left\langle \bar{u}_i'\tau_{i2}^{r'}\right\rangle \\
T_{\text{RES}} &= \frac{d}{dy}\langle \bar{q}\bar{v}'\rangle + \frac{1}{\rho}\frac{d}{dy}\langle \bar{v}'\bar{p}'\rangle - \nu\left\langle \bar{u}_i'\frac{\partial^2 \bar{u}_i'}{\partial x_j \partial x_j}\right\rangle
\end{aligned}$$

Again this allows the velocity gradient $\bar{\phi}(y)$ to be written in terms of the dissipation and transport.

$$\bar{\phi}(y) \equiv \frac{y\kappa}{u_\tau}\frac{d\langle \bar{u}\rangle}{dy} = \frac{y\kappa}{u_\tau}\frac{\tilde{P}_{\text{LES}}}{u_\tau^2 - fy} = \frac{y\kappa}{u_\tau(u_\tau^2 - fy)}\left(\tilde{\epsilon}_{\text{LES}} + T_{\text{SGS}} + T_{\text{RES}}\right) \tag{4.5}$$

From the simulation done with the Mason & Thompson wall model the energy contributions are shown in Figure 4.3.

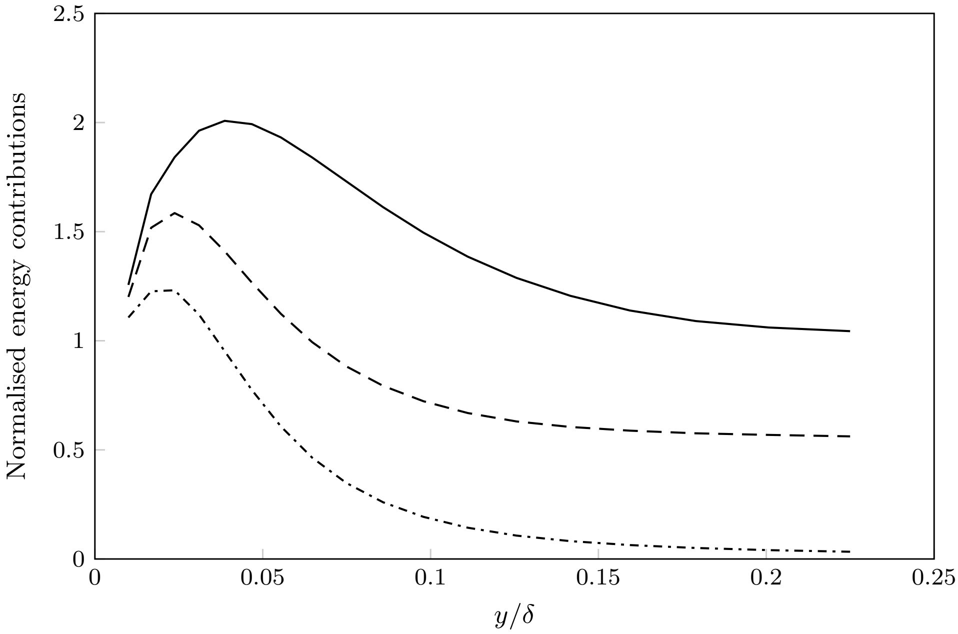


Figure 4.3: Energy contributions for Mason & Thompson wall model. Solid: $\phi(y)$. Dash-dotted: Normalised mean flow SGS dissipation. Dashed: Normalised total subgrid contribution.

Note that inside the inner layer ϕ is determined mostly by subgrid scale contributions. Hence promising that control over the SGS transport term (via the SGS model) influences the normalised mean velocity gradient sufficiently such that the mismatch observed in applying a traditional model can be minimised.

5 A self-adaptive SGS-model

From the analysis of the previous section it is apparent that the transport term involving subgrid-scale motions contributes the most to the normalised mean velocity gradient. In this section a model proposed by Wu & Meyers [11] is derived and discussed. Furthermore it is applied and its performance is compared to that of a traditional model. Note that this model is slightly different from that proposed by Wu & Meyers, since here the flow is not considered to be at Re $\to \infty$. Hence contrary to their analysis the viscous transport term is not neglected.

5.1 Derivation

Considering a Smagorinsky type model of the form

$$\tau_{ij}^r = -2l_s^2|\bar{S}|\bar{S}_{ij}$$

Applying this model to Equation (4.5) yields a relationship between l_s^2 and the normalised mean velocity gradient. First introduce an auxiliary tensor

$$\Psi_{ij} \equiv -2|\bar{S}|\bar{S}_{ij}$$

Such that $\tau_{ij}^r = l_s^2\Psi_{ij}$. Using this, Equation (4.5) becomes

$$\begin{aligned}\bar{\phi}(y) &= \frac{y\kappa}{u_\tau(u_\tau^2 - fy)}\left[\left\langle \frac{\partial l_s^2 \Psi'_{ij}}{\partial x_j}\bar{u}'_i\right\rangle - \left\langle l_s^2 \Psi_{12}\right\rangle \frac{d\langle \bar{u}\rangle}{dy} + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 + T_{\mathrm{RES}}\right] \\ &= \frac{y\kappa}{u_\tau(u_\tau^2 - fy)}\left[\left\langle \Psi'_{ij}\frac{\partial l_s^2}{\partial x_j}\bar{u}'_i\right\rangle + \left\langle l_s^2\frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i\right\rangle - \left\langle l_s^2 \Psi_{12}\right\rangle \frac{d\langle \bar{u}\rangle}{dy} + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 + T_{\mathrm{RES}}\right]\end{aligned}$$

Subsequently a new length scale $\hat{l}_s^2$ is introduced such that

$$\bar{\phi}(y) = \frac{y\kappa}{u_\tau(u_\tau^2 - fy)}\left[\hat{l}_s^2\left(\left\langle \frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i\right\rangle - \langle \Psi_{12}\rangle \frac{d\langle \bar{u}\rangle}{dy}\right) + \frac{d\hat{l}_s^2}{dy}\langle \Psi'_{i2}\bar{u}'_i\rangle + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 + T_{\mathrm{RES}}\right]$$

Re-organising the terms gives an ordinary differential equation

$$A(y)\frac{d\hat{l}_s^2}{dy} + B(y)\hat{l}_s^2 + C(y) = 0$$

Where

$$A(y) = \langle \Psi'_{i2}\bar{u}'_i\rangle, B(y) = \left\langle \frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i\right\rangle - \langle \Psi_{12}\rangle \frac{d\langle \bar{u}\rangle}{dy} \text{ and } C(y) = T_{\mathrm{RES}} + \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 - \frac{u_\tau(u_\tau^2 - fy)\bar{\phi}(y)}{y\kappa}$$

Given a boundary condition this ODE yields an exact solution, however this solution is rather complex. Also a numerical approximation would be computationally expensive. Hence a dimensional analysis is done to see whether the term involving $A(y)$ may be neglected. Consider for convenience $y \approx 0.2\delta$. Such that the following approximation can be made for $\hat{l}_s$

$$\hat{l}_s = C_s\Delta \approx 0.2\Delta$$

I.e. corresponding to the conventional Smagorinsky-Lilly model. From this it follows that

$$\frac{d\hat{l}_s^2}{dy}\langle \Psi'_{i2}\bar{u}'_i\rangle \sim \frac{\hat{l}_s^2}{0.2\delta}\langle \Psi'_{i2}\bar{u}'_i\rangle \sim \hat{l}_s\Delta\left\langle \bar{u}'_i\frac{\Psi'_{i2}}{\delta}\right\rangle$$

Furthermore $\frac{\Psi'_{i2}}{\Delta} \sim \frac{\partial \Psi'_{ij}}{\partial x_j}$, such that

$$\frac{d\hat{l}_s^2}{dy}\langle \Psi'_{i2}\bar{u}'_i\rangle \sim \hat{l}_s\Delta\left\langle \bar{u}'_i\frac{\Psi'_{i2}}{\delta}\right\rangle \ll \hat{l}_s\Delta\left\langle \bar{u}'_i\frac{\Psi'_{i2}}{\Delta}\right\rangle \sim \hat{l}_s^2\left\langle \bar{u}'_i\frac{\partial \Psi'_{ij}}{\partial x_j}\right\rangle$$

Hence the term involving $A(y)$ may be omitted for $y \approx 0.2\delta$. Whether this also holds in the log-region will be confirmed later on with results from applying model. For now it is assumed the term involving $A(y)$ may be neglected. Subsequently taking $\bar{\phi}(y) = 1$, and hence forcing the log-law to hold, an expression for $\hat{l}_s^2$ can be derived

$$\hat{l}_s^2 = -\frac{C(y)}{B(y)} = \frac{\frac{u_\tau(u_\tau^2 - fy)}{y\kappa} - \nu\left(\frac{d\langle \bar{u}\rangle}{dy}\right)^2 - T_{\mathrm{RES}}}{\left\langle \frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i\right\rangle - \langle \Psi_{12}\rangle \frac{d\langle \bar{u}\rangle}{dy}}$$

Using asymptotic analysis it can be shown that a simplified version of this model is Prandtl's mixing length model (When considering $\mathrm{Re} \to \infty$).

Considering a RANS-like simulation (i.e. letting $\bar{u}'_i \to 0$), the adaptive model reduces to

$$\hat{l}_s^2 = -\frac{u_\tau(u_\tau^2 - fy) - \nu\kappa y \left(\frac{d\langle\bar{u}\rangle}{dy}\right)^2}{y\kappa \langle\Psi_{12}\rangle \frac{d\langle\bar{u}\rangle}{dy}}$$

It may be simplified by noting that

$$\langle\Psi_{12}\rangle = \Psi_{12} = -2|\bar{S}|\bar{S}_{12} = -\left(\frac{d\langle\bar{u}\rangle}{dy}\right)^2$$

Such that

$$\hat{l}_s^2 = \frac{u_\tau(u_\tau^2 - fy) - \nu\kappa y \left(\frac{d\langle\bar{u}\rangle}{dy}\right)^2}{y\kappa \left(\frac{d\langle\bar{u}\rangle}{dy}\right)^3} = (\kappa y)^2 \left(1 - \frac{fy}{u_\tau^2} - \frac{\delta_\nu}{\kappa y}\right)$$

It turns out this relationship will provide a good test case for the model later on.

5.2 Applying the model

Now that the adaptive model is derived, it may be implemented into a three-dimensional incompressible fluid solver. Note that the same code was used to run LES simulations with traditional models used in a previous section. It is an extensive `Fortran` code which will be omitted here. However in Appendix E the modifications to the closure models (the subroutine called `CLOSUR`) are shown to the give the reader an idea of how this model was implemented. Before any discretisations can be done, the grid must be defined. A three dimensional grid is used with N_x, N_y, N_z grid points in the x, y and z directions respectively. Quantities like the pressure and the rate-of-strain tensor (or anything that is derived from those) are calculated in the grid points (cell centres). The velocity field however is evaluated at the faces of each of the cells, and hence may be interpreted as in- and outflow of a fluid into a cell. A two dimensional grid is shown in figure 5.1.

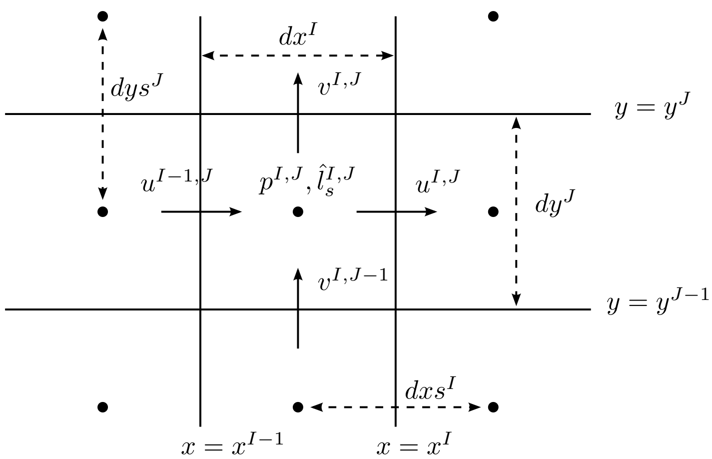


Figure 5.1: The x and y dimensions of the grid.

The grid is non-uniform in the wall-normal direction, such that there are more points close to the wall. The x, y and z directions are labelled I, J and K respectively. They are denoted in superscript to avoid confusion with any tensorial indices. Hence $u_i^{I,J,K} = u_i(x^I, y^J, z^K)$. Note that the mean quantities of the velocity field depend only on the wall-normal direction, hence the superscripts I and K are omitted here. There are N_y wall normal grid points, hence the lower wall is at $y = y^0$ and the upper wall is at $y = y^{N_y}$. The closure model, defined by $\hat{l}_s^2$, is calculated in the cell centres.

Discretisation

Recall that the adaptive model was given by

$$\hat{l}_s^2 = \frac{\frac{u_\tau(u_\tau^2 - fy)}{y\kappa} - \nu\left(\frac{d\langle\bar{u}\rangle}{dy}\right)^2 - T_{\mathrm{RES}}}{\left\langle \frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i \right\rangle - \langle \Psi_{12}\rangle \frac{d\langle\bar{u}\rangle}{dy}}$$

Hence each of the terms occurring in this expression will be discretised and evaluated in the cell centres. Discretised quantities are denoted by $\frac{\delta}{\delta x_i}$.

(I) First of all the friction velocity u_τ is discretised:

$$u_\tau^2 = \frac{\tau_w}{\rho} = \nu\left(\frac{\delta\langle\bar{u}\rangle}{\delta y}\right)_{y=0} = \nu\frac{\langle\bar{u}\rangle^1}{\frac{1}{2}dy^1}$$

(II) Furthermore the mean pressure gradient is discretised

$$f^{I,J,K} = -\frac{1}{\rho}\frac{\delta\langle\bar{p}\rangle}{\delta x}^{I,J,K} = -\frac{1}{\rho}\frac{\langle\bar{p}\rangle^{I+1,J,K} - \langle\bar{p}\rangle^{I-1,J,K}}{dxs^I + dxs^{I-1}}$$

(III) A rather cumbersome term is the following

$$\left\langle \frac{\partial \Psi'_{ij}}{\partial x_j}\bar{u}'_i \right\rangle^J$$

For $j = 1$ it is discretised as

$$\frac{\delta\Psi'_{i1}}{\delta x}^{I,J,K} = \frac{\Psi'^{I+1,J,K}_{i1} - \Psi'^{I-1,J,K}_{i1}}{dxs^I + dxs^{I-1}}$$

And similarly for $j = 2, 3$. Note that $\bar{u}'|_c^{I,J,K}$ is the value in the cell centre, hence it is equal to

$$\bar{u}'|_c^{I,J,K} = \frac{1}{2}\left(\bar{u}'^{I-1,J,K} + \bar{u}'^{I,J,K}\right)$$

(IV) The second term in the denominator is

$$\langle\Psi_{12}\rangle\frac{d\langle\bar{u}\rangle}{dy}^J$$

The auxiliary tensor may be computed in the cell centres by using the rate-of-strain tensor. Subsequently it is averaged in the x and y directions as well as in time. The mean velocity gradient is set to equal the law of the wall.

(V) The mean flow viscous dissipation is discretised similarly to how the mean flow SGS dissipation is discretised.

(VI) Finally the resolved turbulent transport term will be discretised.

$$T_{\mathrm{RES}} = \frac{d}{dy}\langle\bar{q}\bar{v}'\rangle + \frac{1}{\rho}\frac{d}{dy}\langle\bar{v}'\bar{p}'\rangle - \nu\left\langle \bar{u}'_i\frac{\partial^2\bar{u}'_i}{\partial x_j\partial x_j}\right\rangle$$

This is how it was defined in Section 4.2, in continuous form this is equal to

$$T_{\mathrm{RES}} = \left\langle \bar{u}'_i\frac{\partial\bar{u}'_i\bar{u}'_j}{\partial x_j}\right\rangle + \frac{1}{\rho}\left\langle \bar{u}'_i\frac{\partial\bar{p}'}{\partial x_i}\right\rangle - \nu\left\langle \bar{u}'_i\frac{\partial^2\bar{u}'_i}{\partial x_j\partial x_j}\right\rangle \tag{5.1}$$

However these two formulations are not equal in discrete form. Since Equation (5.1) follows directly from the derivation of the turbulent kinetic energy equation for LES, this form is preferable.

The first term is discretised in the following way, consider $(i,j) = (1,2)$.

$$\frac{\delta \bar{u}'\bar{v}'^{\,I,J}}{\delta y} = \frac{\left[(\bar{u}'^{I-1,J+1} + \bar{u}'^{I,J+1})(\bar{v}'^{I,J} + \bar{v}'^{I,J+1}) - (\bar{u}'^{I-1,J-1} + \bar{u}'^{I,J-1})(\bar{v}'^{I,J-2} + \bar{v}'^{I,J-1})\right]}{4(dys^J + dys^{J-1})}$$

All for $z = z^K$. Furthermore the second term is discretised straightforwardly. Finally consider the viscous transport term

$$\nu \left\langle \bar{u}_i' \frac{\partial^2 \bar{u}_i'}{\partial x_j \partial x_j} \right\rangle$$

To show how the second order derivative is discretised, once again consider $(i,j) = (1,2)$.

$$\frac{\delta^2 \bar{u}'}{\delta y^2} = \frac{1}{2dy^J}\left[\frac{(\bar{u}'^{I-1,J+1} + \bar{u}'^{I,J+1}) - (\bar{u}'^{I-1,J} + \bar{u}'^{I,J})}{dys^J} - \frac{(\bar{u}'^{I-1,J} + \bar{u}'^{I,J}) - (\bar{u}'^{I-1,J-1} + \bar{u}'^{I,J-1})}{dys^{J-1}}\right]$$

The superscript for the span wise direction is omitted. Everything is evaluated at $z = z^K$.

Note that the ensemble average $\langle . \rangle$ in discrete form is replaced by a combination of both time and spatial averaging. Where the spatial average is taken in the x and z directions, i.e. the directions in which the flow is statistically invariant.

Normalised mean velocity gradient

Even though $\bar{\phi}(y)$ was forced to equal one to agree to the log-law, it turns out that near the wall, this will cause discretisation errors near the wall [11]. To analyse this, the discretisation of the normalised mean velocity gradient is considered.

$$\frac{y\kappa}{u_\tau}\frac{\delta \langle \bar{u} \rangle}{\delta y}$$

Consider any discretisation scheme, the discretised mean velocity gradient may be written as

$$\frac{\delta \langle \bar{u} \rangle}{\delta y} = \frac{d \langle \bar{u} \rangle}{dy} + c_1 \Delta_y \frac{d^2 \langle \bar{u} \rangle}{dy^2} + c_2 \Delta_y^2 \frac{d^3 \langle \bar{u} \rangle}{dy^3} + \dots \tag{5.2}$$

Hence when using a central finite difference scheme, $c_1 = 0$ and $c_2 = \frac{1}{6}$. However any discretisation scheme may be considered here. Using the law of the wall (2.12), the following holds

$$\frac{d^n \langle \bar{u} \rangle}{dy^n} = (-1)^{n-1} \frac{u_\tau}{\kappa} \frac{(n-1)!}{y^n}$$

So Equation (5.2) becomes

$$\frac{\delta \langle \bar{u} \rangle}{\delta y} = \frac{d \langle \bar{u} \rangle}{dy} - c_1 \Delta_y \frac{u_\tau}{\kappa}\frac{1}{y^2} + c_2 \Delta_y^2 \frac{u_\tau}{\kappa}\frac{2}{y^3} + \dots$$

For convenience a new wall distance is defined: $d \equiv \frac{y}{\Delta_y}$, such that the discretised mean shear can be written as

$$\frac{\delta \langle \bar{u} \rangle}{\delta y} = \frac{d \langle \bar{u} \rangle}{dy} + \frac{u_\tau}{\kappa} \sum_{k=1}^{\infty} (-1)^k \frac{c_k k! \Delta_y^k}{y^{k+1}} = \frac{d \langle \bar{u} \rangle}{dy} + \frac{u_\tau}{\Delta_y \kappa} \sum_{k=1}^{\infty} (-1)^k \frac{c_k k!}{d^{k+1}}$$

Hence the relative error is given by

$$\frac{\frac{\delta\langle\bar{u}\rangle}{\delta y}-\frac{d\langle\bar{u}\rangle}{dy}}{\frac{d\langle\bar{u}\rangle}{dy}}=\sum_{k=1}^{\infty}(-1)^k(-1)^k\frac{c_k k!}{d^k}$$

From this it follows that the relative error becomes large for $d<1$. To avoid this, a logarithmic mean velocity profile is presumed. Hence $\langle\bar{u}\rangle=\frac{u_\tau}{\kappa}\ln y^+ + B$. This leads to the following approximation

$$\frac{\delta\left\langle\bar{u}\right\rangle}{\delta y}^J=\frac{u_\tau}{\kappa}\frac{\ln y^J-\ln y^{J-1}}{dy^J}$$

Hence instead of using $\bar{\phi}(y)=1$, the following approximation is used

$$\bar{\phi}(y)=\frac{y\kappa}{u_\tau}\frac{\delta\left\langle\bar{u}\right\rangle}{\delta y}^J=y\frac{\ln y^J-\ln y^{J-1}}{dy^J}$$

However this would still force a log-profile even close to the wall, which is not as desired. Hence on the first 2 grid points ($y^+<5$), the law of the wall for the viscous sublayer is enforced:

$$u^+=y^+$$

This relates to the normalised mean velocity gradient in the following way

$$\begin{aligned}\bar{\phi}(y)&=\frac{y\kappa}{u_\tau}\frac{d\left\langle\bar{u}\right\rangle}{dy}\\&=\frac{y\kappa u_\tau}{\nu}\end{aligned}$$

Blending

When using the adaptive model with the previously discussed normalised mean velocity gradient, it still only holds in the inner layer. Hence at some distance from the wall a standard model must be used. From the theory it follows that the inner layer ends at $y=0.1\delta$, hence this point is used to start blending from the adaptive to the traditional model around $y=0.1\delta$. Blending is done on 5 points, using the cosine as a blending function.

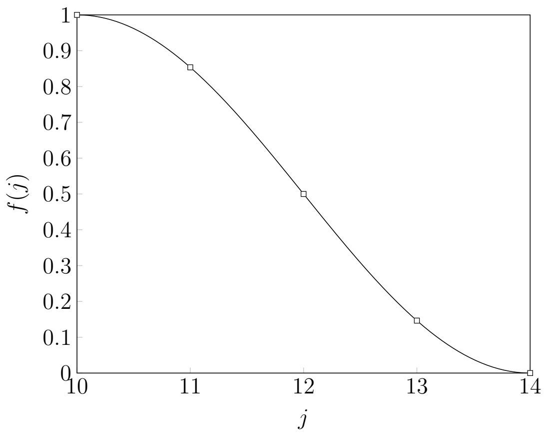


Figure 5.2: Blending function

I.e. both the Smagorinsky length scale corresponding to the traditional model and the dynamic model are calculated and subsequently averaged using the blending function.

5.3 Results

The adaptive model was applied using the 14-th grid point as a blending position. This point corresponds to $y/\delta \approx 0.11$, hence lying inside the theoretical inner layer. The simulation was ran using a Reynolds number of 22600. The velocity profile obtained from this simulation is the following:

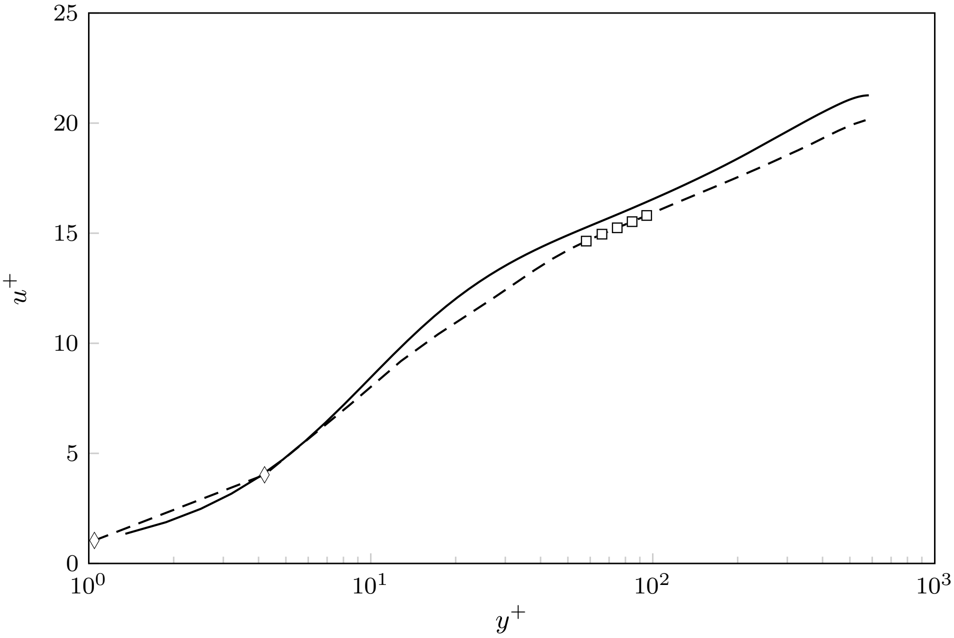


Figure 5.3: Velocity profile using the dynamic model where blending was done at $j = 14$ (dashed). ($\Diamond$) denotes grid points where ϕ is forced to agree with the law of the wall inside the viscous layer. ($\Box$) are grid points where blending is applied. Solid: DNS data of Kim et al. [1].

More interesting however is the resulting normalised mean velocity gradient

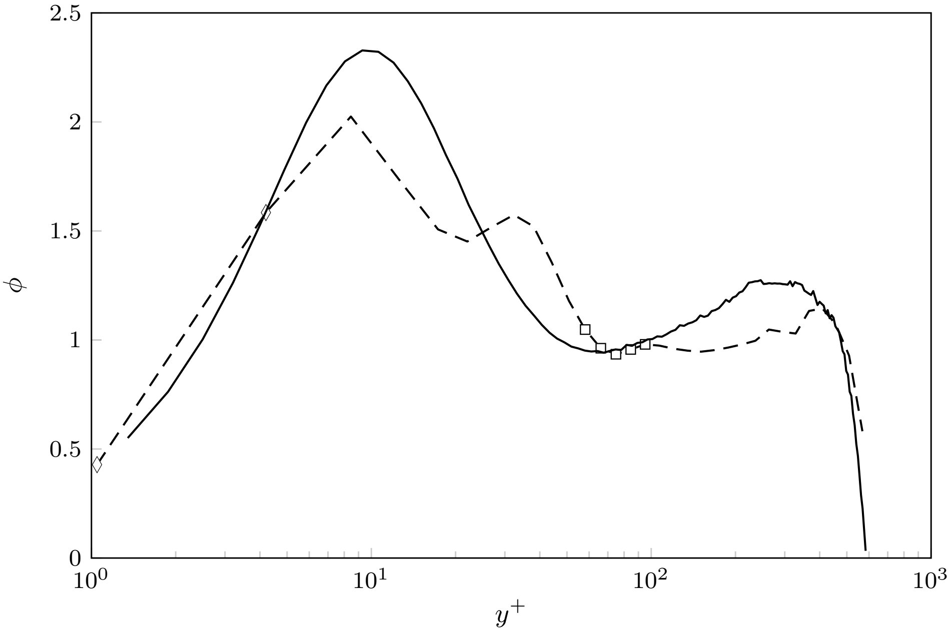


Figure 5.4: Normalised mean velocity gradient, using the dynamic model where blending was done at $j = 14$ (dashed). ($\Diamond$) denotes grid points where ϕ is forced to agree with the law of the wall inside the viscous layer. ($\Box$) are grid points where blending is applied. Solid: DNS data of Kim et al. [1].

This shows first of all that forcing the normalised mean velocity gradient in the viscous sublayer works fine, except that another point might be added (third grid point). Furthermore it seems that the normalised mean velocity gradient tends to 1 a bit too far into the channel, hence the blending position should be shifted slightly to the left.

However before these modifications are applied, the model is tested in a different setup as well. First of all recall that in the derivation of this model (Section 5.1) it was mentioned that in a RANS like simulation (letting $\bar{u}_i' = 0$) the length scale should simplify to

$$\hat{l}_s^2 = (\kappa y)^2 \left(1 - \frac{fy}{u_\tau^2} - \frac{\delta_\nu}{\kappa y}\right) \tag{5.3}$$

Hence when forcing to velocity field to exactly agree to the log-law (throughout the entire half-height of the channel) and letting all the fluctuating velocity quantities equal zero, this is what the dynamic model should give as a length scale. So the `Fortran` code was modified slightly to read a perfect logarithmic velocity profile (with $u_\tau = 1$) and the corresponding length scale calculated by the model was compared to that mentioned in Equation (5.3). The relative error of the length scale returned by the model is shown in Figure 5.5.

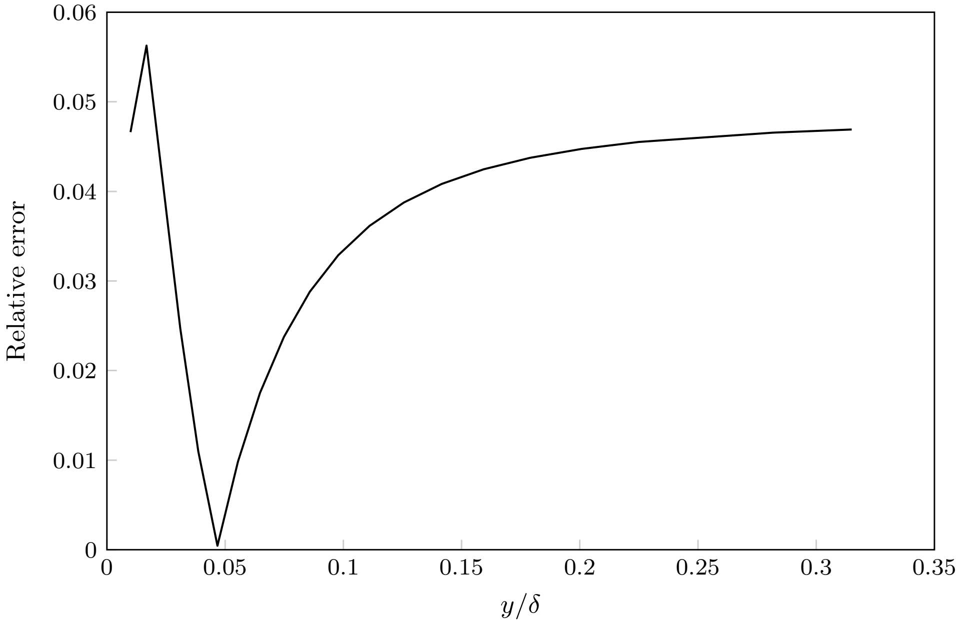


Figure 5.5: The relative error of the length scale returned by the model.

Note that when the friction velocity is forced to equal 1, instead of linearly approximating it, the length scale matches perfectly. Hence the discretisation of u_τ could be improved. However since the relative error is small, this is left for future endeavours.

Next the improvements mentioned above are implemented into the dynamic model. The simulation is run again, the results are as follows. Grey colour denotes results of the first attempt.

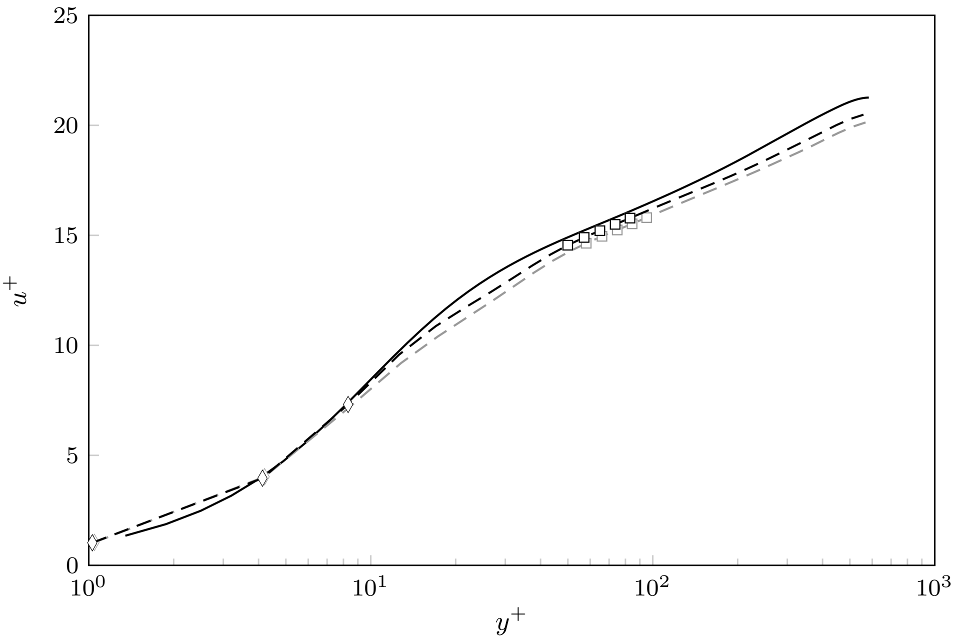


Figure 5.6: Velocity profile using the dynamic model where blending was done at $j = 13$ (dashed). ($\Diamond$) denotes grid points where ϕ is forced to agree with the law of the wall inside the viscous layer. ($\Box$) are grid points where blending is applied. Solid: DNS data of Kim et al. [1].

And the resulting normalised mean velocity gradient

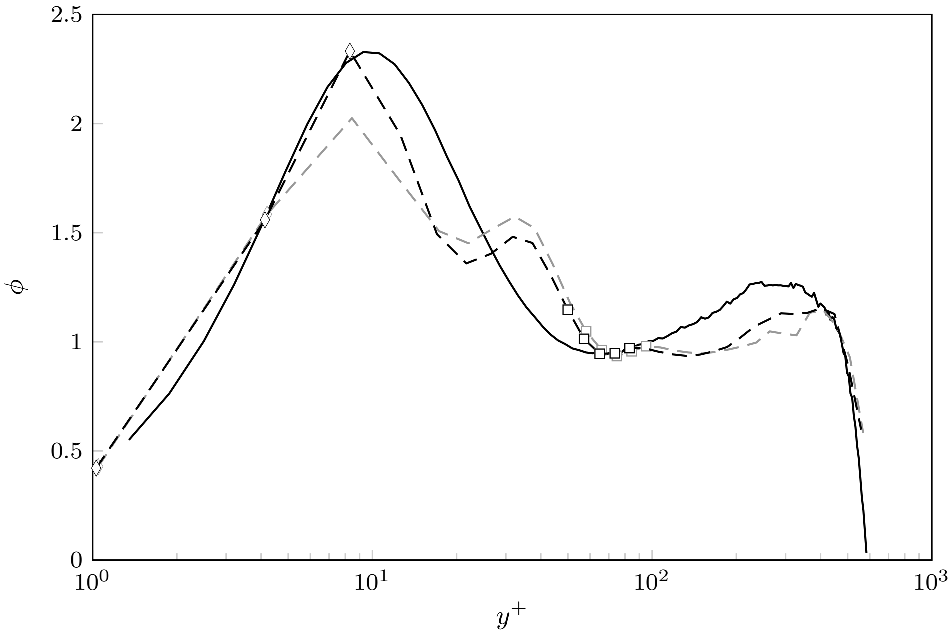


Figure 5.7: Normalised mean velocity gradient, using the dynamic model where blending was done at $j = 13$ (dashed). ($\Diamond$) denotes grid points where ϕ is forced to agree with the law of the wall inside the viscous layer. ($\Box$) are grid points where blending is applied. Solid: DNS data of Kim et al. [1].

The normalised mean velocity gradient gives the most insightful relationship to analyse the improvements made over the the first attempt. The viscous sublayer now shows excellent agreement with $u^+ = y^+$. Moving the blending point to the left did not seem to have much influence on the normalised mean velocity gradient, except that the 'bump' around $y^+ = 300$ seems to agree better. One, so far unexplained, artefact occurs around $y^+ = 30$. Whether this is due to an error or whether this can be explained by studying the energy contributions is unknown so far. Perhaps studying this artefact may lead to further improvements.

Finally large scale figures of both the normalised mean velocity gradient as the velocity profile are shown summarising the results from this report. This includes a dynamic model based on the invariants of the rate-of-strain tensor, which is added for comparison [9].

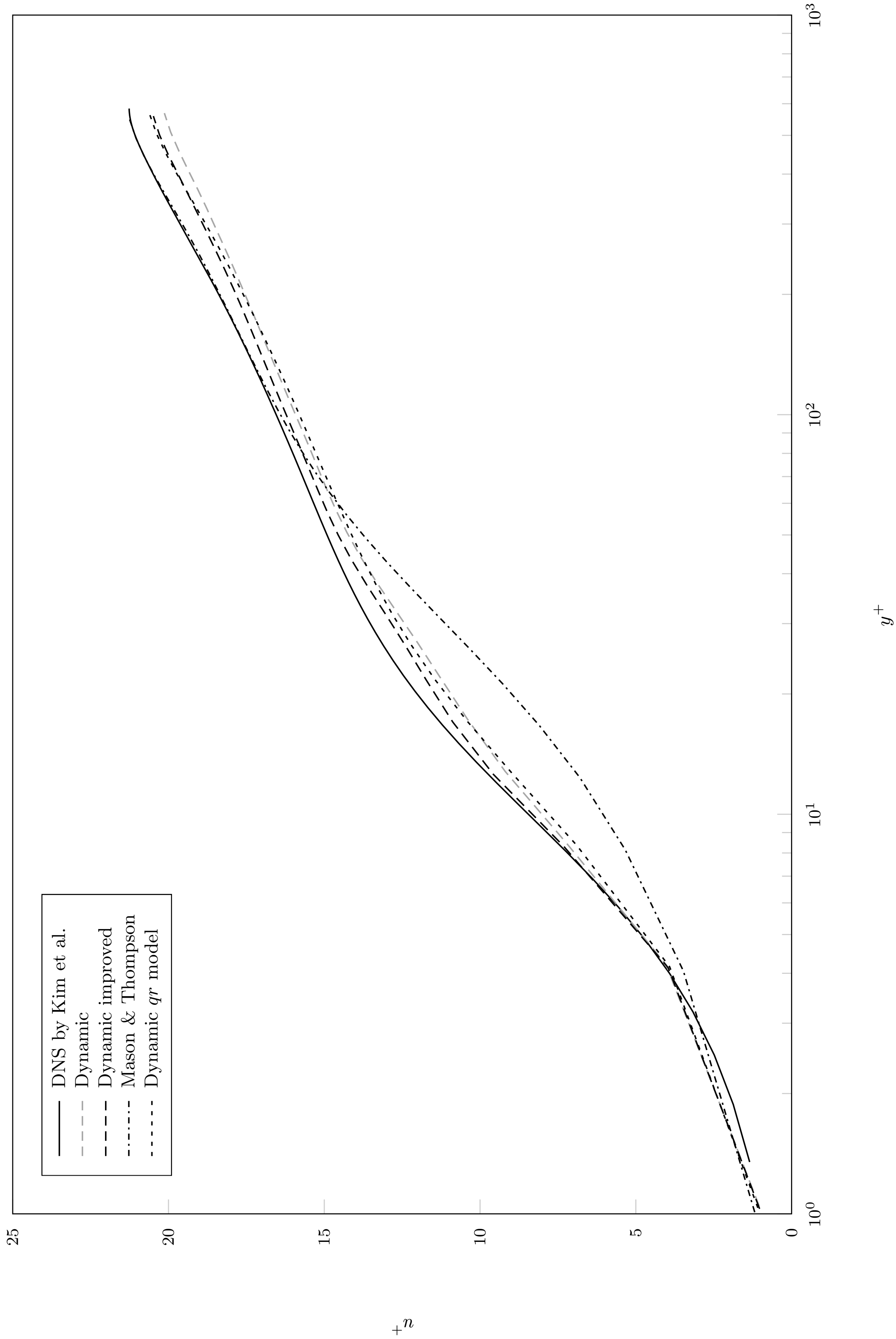


Figure 5.8: Velocity profile shown for several SGS models

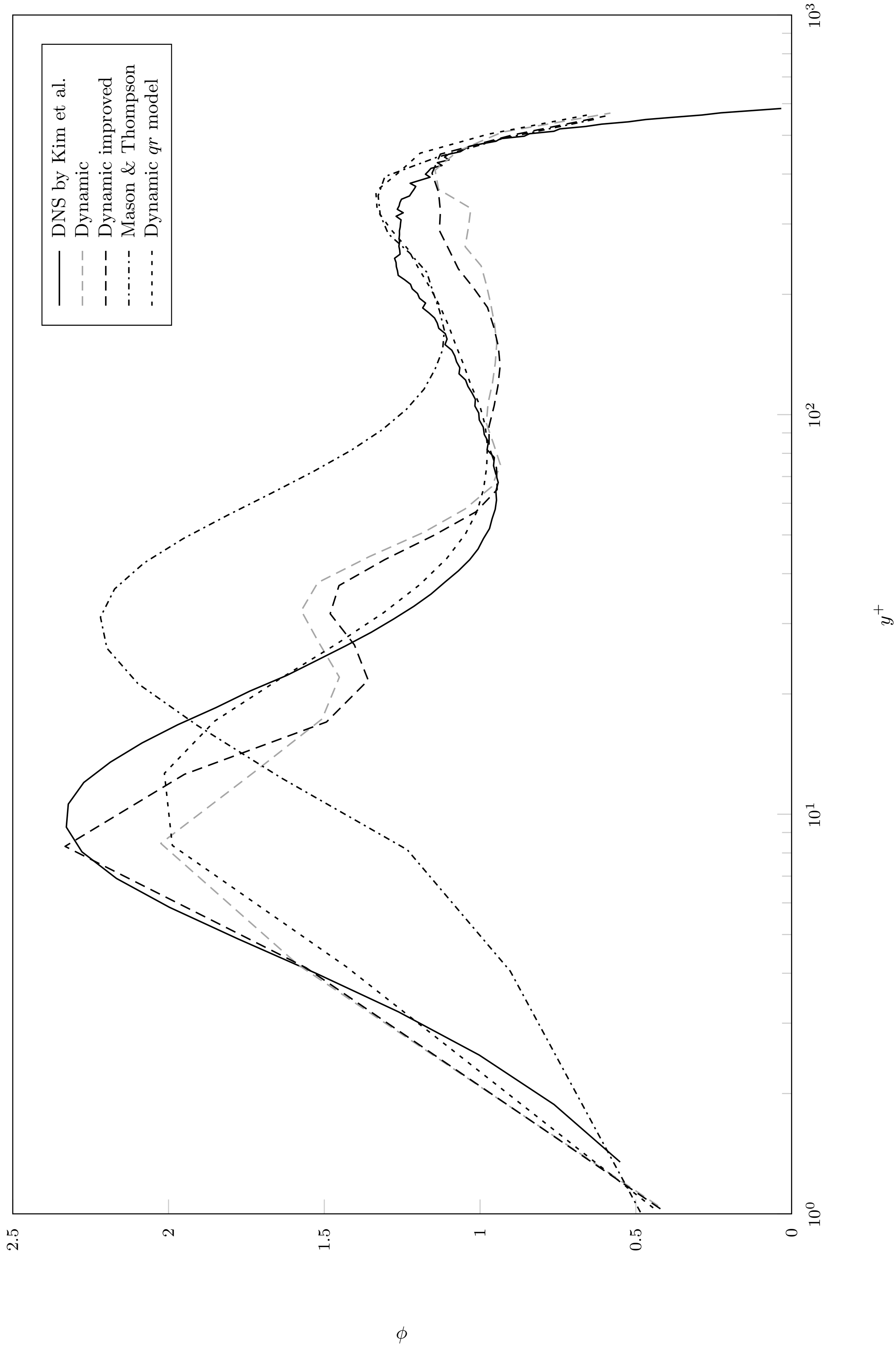


Figure 5.9: Normalised mean velocity gradient shown for several SGS models

6 Concluding remarks

In this report a brief overview of channel flow was given. This leading up to large eddy simulation which inevitably lead to the discussion of several traditional wall models. One of the issues with such a model, the Mason & Thompson wall model, was discussed. The mismatch of the normalised mean velocity gradient was recognised and analysed. We realised that mostly the dissipation of the subgrid scales contributed to this velocity gradient in the inner layer. Hence why a model by Wu & Meyers was derived to dynamically change the Smagorinsky length scale such that it would force the normalised mean velocity gradient to be approximately equal one inside the log layer. Furthermore this model was modified to also work with relatively low Reynolds number flow. Further adjustments were made such that the normalised mean velocity gradient would also agree to DNS in the viscous sublayer.

Results from this model look promising. It performs much better than traditional models, without the need of a lot of tweaking. However there are still some issues. For future research the discretisation of the friction velocity could be done by integrating the momentum balance to reach a higher accuracy. Finally the noticed bump in the normalised mean velocity gradient around $y^+ = 30$ requires further investigation.

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Appendices

A Einstein notation

Einstein's summation convention is a useful shorthand notation for writing summations. It is based on repeated indices. Whenever in a multiplication or fraction an index is repeated, it implies a sum. Some examples:

$$u_i \frac{\partial u_j}{\partial x_i} = \sum_{i=1}^{n} u_i \frac{\partial u_j}{\partial x_i}$$

but also

$$\frac{\partial u_i}{\partial x_i} = \sum_{i=1}^{n} \frac{\partial u_i}{\partial x_i} = \nabla \cdot \mathbf{u}$$

The summation maximum n is always known from the context in which it appears. Note that it is almost always equal to three.

B Filter properties

The linearity and scalar multiplication properties follow directly from the definition of a filter , as was given in Equation (3.1). The third property however, which states that filtering commutes with taking a derivative, holds only in special cases and requires some attention. Let $G(\mathbf{r}, \mathbf{x})$ be a kernel. Then taking a spatial derivative of a filtered function $\overline{f(\mathbf{x})}$ becomes

$$\begin{aligned}
\frac{\partial \overline{f(\mathbf{x})}}{\partial x_j} &= \frac{\partial}{\partial x_j} \int_\Omega G(\mathbf{r}, \mathbf{x}) f(\mathbf{x} - \mathbf{r}) d\mathbf{r} \\
&= \int_\Omega \frac{\partial}{\partial x_j} \left[G(\mathbf{r}, \mathbf{x}) f(\mathbf{x} - \mathbf{r}) \right] d\mathbf{r} \\
&= \int_\Omega G(\mathbf{r}, \mathbf{x}) \frac{\partial f(\mathbf{x} - \mathbf{r})}{\partial x_j} d\mathbf{r} + \int_\Omega \frac{\partial G(\mathbf{r}, \mathbf{x})}{\partial x_j} f(\mathbf{x} - \mathbf{r}) d\mathbf{r} \\
&= \overline{\frac{\partial f(\mathbf{x})}{\partial x_j}} + \int_\Omega \frac{\partial G(\mathbf{r}, \mathbf{x})}{\partial x_j} f(\mathbf{x} - \mathbf{r}) d\mathbf{r}
\end{aligned}$$

I.e. if a spatial filter is invariant under translation $G(\mathbf{r}, \mathbf{x}) = G(\mathbf{r})$ then taking a spatial derivative commutes with filtering.

C Linearity of law of the wall in the viscous sublayer

Consider u', v', w', the fluctuating parts of the velocity field, in a fixed x, z coordinate. Then for small y, let u' and v' be approximated as follows

$$u' = a_1 + b_1 y + c_1 y^2$$

$$v' = a_2 + b_2 y + c_2 y^2$$

From the boundary conditions (no-slip and no permuation) at $y = 0$ it follows that

$$u'|_{y=o} = v'|_{y=0} = 0$$

So $a_1 = b_1 = 0$. Also from the same boundary conditions the following can be derived

$$\left(\frac{\partial u'}{\partial x}\right)_{y=0} = \left(\frac{\partial w'}{\partial z}\right)_{y=0} = 0$$

Hence from the continuity of the fluctuating part of the velocity field it follows that

$$b_2 = \left(\frac{\partial v'}{\partial y}\right)_{y=0} = 0$$

From this analysis an estimate for $\langle u'v' \rangle$ can be made

$$\langle u'v' \rangle = \langle b_1 c_2 \rangle y^3 + \ldots$$

Which can be written as

$$\langle u'v' \rangle = -\sigma u_\tau^2 {y^+}^3 + \ldots \tag{C.1}$$

Where σ is a dimensionless constant. Recall from Section 2.2

$$\tau(y) = \rho\nu \frac{d\langle u \rangle}{dy} - \rho \langle u'v' \rangle \tag{C.2}$$

$$= \tau_w \left(1 - \frac{y}{\delta}\right) \tag{C.3}$$

Such that from Equations (C.2) & (C.3) it follows that

$$\frac{d\langle u \rangle}{dy} = \frac{\tau_w}{\rho\nu} - \frac{\tau_w}{\delta\rho\nu} y + \frac{\langle u'v' \rangle}{\nu}$$

From which up to the fourth order derivative of $\langle u \rangle$ can be derived (using Equation (C.1))

$$\begin{aligned}
\frac{d^2\langle u \rangle}{dy^2} &= -\frac{\tau_w}{\delta\rho\nu} + \frac{1}{\nu}\frac{d}{dy}\left(-\sigma u_\tau^2 {y^+}^3\right) \\
&= -\frac{\tau_w}{\delta\rho\nu} + \frac{1}{\nu}\frac{d}{dy^+}\left(-\sigma u_\tau^2 {y^+}^3\right)\frac{dy^+}{dy} \\
&= -\frac{\tau_w}{\delta\rho\nu} + \frac{u_\tau}{\nu^2}\left(-3\sigma u_\tau^2\right) y^+ \\
\frac{d^3\langle u \rangle}{dy^3} &= \frac{-6\sigma u_\tau^4}{\nu^3} y^+ \\
\frac{d^4\langle u \rangle}{dy^4} &= \frac{-6\sigma u_\tau^5}{\nu^4}
\end{aligned}$$

Hence using a Taylor series expansion of $\langle u \rangle$ the following estimate can be obtained

$$\langle u \rangle \approx \langle u \rangle_{y=0} + \left(\frac{d\langle u \rangle}{dy}\right)_{y=0} y + \frac{1}{2}\left(\frac{d^2\langle u \rangle}{dy^2}\right)_{y=0} y^2 + \frac{1}{6}\left(\frac{d^3\langle u \rangle}{dy^3}\right)_{y=0} y^3 + \frac{1}{24}\left(\frac{d^4\langle u \rangle}{dy^4}\right)_{y=0} y^4$$

Finally an estimate for u^+ arises

$$\begin{aligned}
u^+ &= \frac{\langle u \rangle}{u_\tau} \\
&\approx \frac{1}{u_\tau}\left[\frac{u_\tau^2}{\nu}\frac{\nu}{u_\tau} y^+ - \frac{u_\tau^2}{2\delta\nu}\frac{\nu^2}{u_\tau^2}{y^+}^2 + \frac{1}{24}\frac{-6\sigma u_\tau^5}{\nu^4}\frac{\nu^4}{u_\tau^4}{y^+}^4\right] \\
&= y^+ - \frac{1}{2\mathrm{Re}_\tau}{y^+}^2 - \frac{1}{4}\sigma {y^+}^4
\end{aligned}$$

So for large Re_τ the law of the wall in the viscous sublayer yields

$$u^+ = y^+ - \frac{1}{4}\sigma {y^+}^4 = f_w(y^+)$$

Hence the law of the wall in the viscous sublayer is linear up to third order approximation.

D Turbulent kinetic energy equations

The turbulent kinetic energy equations are used for the analysis of the velocity gradient overshoot. The derivation of the equations is a rather straightforward calculation, however it might initially not be obvious to derive in the way it is done here. In the end an equation in terms of the turbulent kinetic energy is obtained.

D.1 DNS

The turbulent kinetic energy equations follow from fluctuating part of the NS momentum equation for incompressible and stationary flow. Recall the NS momentum equation

$$u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{D.1}$$

Hence the mean of Equation (D.1) is given by

$$\frac{\partial \langle u_j u_i \rangle}{\partial x_j} = -\frac{1}{\rho}\left\langle \frac{\partial p}{\partial x_i} \right\rangle + \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_j \partial x_j}$$

Where the continuity equation is used together with the fact that taking the mean and differentiating commute. So from this the fluctuating part of the NS equation can be derived

$$\frac{\partial}{\partial x_j}\left[u_i u_j - \langle u_j u_i \rangle\right] = -\frac{1}{\rho}\frac{\partial p'}{\partial x_i} + \nu \frac{\partial^2 u_i'}{\partial x_j \partial x_j} \tag{D.2}$$

Where p' is the fluctuating part of p. The LHS can be written in the following way

$$\begin{aligned}
\frac{\partial}{\partial x_j}\left[u_i u_j - \langle u_j u_i \rangle\right] &= \frac{\partial}{\partial x_j}\left[(\langle u_i \rangle + u_i')(\langle u_j \rangle + u_j') - \left\langle (\langle u_i \rangle + u_i')(\langle u_j \rangle + u_j') \right\rangle\right] \\
&= \frac{\partial}{\partial x_j}\left[u_i' u_j' - \langle u_i' u_j' \rangle + u_i' \langle u_j \rangle + u_j' \langle u_i \rangle\right]
\end{aligned}$$

Furthermore Equation (D.2) is multiplied by u_i' and subsequently the mean is taken of that result, this leads to

$$\left\langle u_i' \frac{\partial}{\partial x_j}\left[u_i' u_j' - \langle u_i' u_j' \rangle + u_i' \langle u_j \rangle + u_j' \langle u_i \rangle\right] \right\rangle = -\frac{1}{\rho}\frac{\partial \langle u_i' p' \rangle}{\partial x_i} + \nu \left\langle u_i' \frac{\partial^2 \langle u_i \rangle}{\partial x_j \partial x_j} \right\rangle \tag{D.3}$$

Considering the LHS only

$$\underbrace{\left\langle u_i' \frac{\partial}{\partial x_j}(u_i' u_j') \right\rangle}_{\mathrm{I}} - \underbrace{\left\langle u_i' \frac{\partial}{\partial x_j}\langle u_i' u_j' \rangle \right\rangle}_{\mathrm{II}} + \underbrace{\left\langle u_i' \frac{\partial}{\partial x_j}(u_i' \langle u_j \rangle) \right\rangle}_{\mathrm{III}} + \underbrace{\left\langle u_i' \frac{\partial}{\partial x_j}(u_j' \langle u_i \rangle) \right\rangle}_{\mathrm{IV}}$$

I:

$$\begin{aligned}
\left\langle u_i' \frac{\partial}{\partial x_j}(u_i' u_j') \right\rangle &= \frac{1}{2}\left\langle u_i' \frac{\partial}{\partial x_j}(u_i' u_j') \right\rangle + \frac{1}{2}\left\langle u_i' u_j' \frac{\partial}{\partial x_j}(u_i') \right\rangle \\
&= \frac{1}{2}\left\langle \frac{\partial}{\partial x_j}(u_i' u_i' u_j') \right\rangle \\
&= \frac{d}{dy}\langle q v' \rangle
\end{aligned}$$

Where in the last step the statistical one-dimensionality of fully developed flow is used. Also, q is defined as

$$q \equiv \frac{u_i' u_i'}{2}$$

II:

$$\begin{aligned}\left\langle u_i' \frac{\partial}{\partial x_j} \left\langle u_i' u_j' \right\rangle \right\rangle &= \left\langle u_i' \right\rangle \frac{\partial}{\partial x_j} \left\langle u_i' u_j' \right\rangle \\ &= 0\end{aligned}$$

III:

$$\begin{aligned}\left\langle u_i' \frac{\partial}{\partial x_j} \left(u_i' \left\langle u_j \right\rangle \right) \right\rangle &= \left\langle u_i' \frac{d}{dy} \left(u_i' \left\langle v \right\rangle \right) \right\rangle \\ &= 0 \text{ , since } \left\langle v \right\rangle = 0\end{aligned}$$

IV:

$$\begin{aligned}\left\langle u_i' \frac{\partial}{\partial x_j} \left(u_j' \left\langle u_i \right\rangle \right) \right\rangle &= \left\langle u_i' u_j' \frac{\partial}{\partial x_j} \left\langle u_i \right\rangle \right\rangle \\ &= \left\langle u_i' u_j' \right\rangle \frac{\partial}{\partial x_j} \left\langle u_i \right\rangle \\ &= \left\langle u' v' \right\rangle \frac{d \left\langle u \right\rangle}{dy} \text{ , since } \left\langle v \right\rangle = \left\langle w \right\rangle = 0\end{aligned}$$

Furthermore the second RHS term of Equation (D.3) can be written as

$$\begin{aligned}\nu \left\langle u_i' \frac{\partial^2 u_i'}{\partial x_j \partial x_j} \right\rangle &= \nu \left\langle \frac{\partial}{\partial x_j} \left(u_i' \frac{\partial}{\partial x_j} u_i' \right) \right\rangle - \nu \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right\rangle \\ &= \nu \left\langle \frac{\partial}{\partial x_j} \left(u_i' \frac{\partial u_i'}{\partial x_j} \right) \right\rangle - \nu \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right\rangle \\ &= \nu \frac{d^2 k}{dy^2} - \nu \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right\rangle\end{aligned}$$

Where

$$k \equiv \frac{\left\langle u_i' u_i' \right\rangle}{2}$$

Hence in total, Equation (D.3) leads to the turbulent kinetic energy equation

$$0 = -\frac{d}{dy} \left\langle q v' \right\rangle - \left\langle u' v' \right\rangle \frac{d \left\langle u \right\rangle}{dy} - \frac{1}{\rho} \frac{d}{dy} \left\langle v' p' \right\rangle + \nu \frac{d^2 k}{dy^2} - \nu \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right\rangle$$

D.2 LES

The derivation for the turbulent kinetic energy equation for LES is very similar to the one for DNS, hence some steps will be omitted. Similar to the DNS case the fluctuating part of the NS equations is the starting point. However for LES, the filtered NS equations are considered.

Recall the filtered NS Equation (3.7) (for stationary flow).

$$\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\nu \bar{S}_{ij} - \tau_{ij}^r \right)$$

Similarly to the derivation of the turbulent kinetic energy equation, the fluctuating part of the filtered NS equation is considered.

$$\frac{\partial \bar{u}_i \bar{u}_j - \langle \bar{u}_i \bar{u}_j \rangle}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}'}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\nu \bar{S}'_{ij} - \tau^{r'}_{ij}\right) \tag{D.4}$$

Now Equation (D.4) is multiplied by $\bar{u}'_i$ and subsequently the mean of this result is taken. The derivation of the LHS is analogous to it's DNS counterpart, hence it will be omitted here. The term involving the fluctuating part of the residual stress tensor becomes

$$\begin{aligned} -\left\langle \bar{u}'_i \frac{\partial \tau^{r'}_{ij}}{\partial x_j} \right\rangle &= -\frac{\partial}{\partial x_j}\left\langle \bar{u}'_i \tau^{r'}_{ij} \right\rangle + \left\langle \frac{\partial \bar{u}'_i}{\partial x_j} \tau^{r'}_{ij} \right\rangle \\ &= -\frac{d}{dy}\left\langle \bar{u}'_i \tau^{r'}_{i2} \right\rangle + \left\langle \frac{\partial \bar{u}'_i}{\partial x_j} \tau^{r'}_{ij} \right\rangle \end{aligned}$$

Hence the turbulent kinetic energy equation for LES becomes

$$0 = -\frac{d}{dy}\langle \bar{q}\bar{v}' \rangle - \langle \bar{u}'\bar{v}' \rangle \frac{d\langle \bar{u} \rangle}{dy} - \frac{1}{\rho}\frac{d}{dy}\langle \bar{v}'\bar{p}' \rangle - \frac{d}{dy}\left\langle \bar{u}'_i \tau^{r'}_{i2} \right\rangle + \left\langle \frac{\partial \bar{u}'_i}{\partial x_j}\tau^{r'}_{ij} \right\rangle + \nu\left\langle \bar{u}'_i \frac{\partial^2 \bar{u}'_i}{\partial x_j \partial x_j} \right\rangle$$

Where

$$\bar{q} \equiv \frac{\bar{u}'_i \bar{u}'_i}{2}$$

D.3 Splitting the pseudo-dissipation

This is a straightforward calculation. It relies on writing the fluctuating velocity gradient in terms of its symmetric and anti-symmetric part

$$S'_{ij} \equiv \frac{1}{2}\left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right)$$

And

$$A'_{ij} \equiv \frac{1}{2}\left(\frac{\partial u'_i}{\partial x_j} - \frac{\partial u'_j}{\partial x_i}\right)$$

Hence the pseudo-dissipation can be written as

$$\begin{aligned} \nu\left\langle \frac{\partial u'_i}{\partial x_j}\frac{\partial u'_i}{\partial x_j} \right\rangle &= \nu\left\langle \left(S'_{ij} + A'_{ij}\right)^2 \right\rangle \\ &= \nu\left\langle S'_{ij}S'_{ij} \right\rangle + 2\nu\left\langle S'_{ij}A'_{ij} \right\rangle + \nu\left\langle A'_{ij}A'_{ij} \right\rangle \end{aligned}$$

As can be easily seen, the term concerning the product of the symmetric and anti-symmetric part equals zero. The third term yields

$$\begin{aligned} \nu\left\langle A'_{ij}A'_{ij} \right\rangle &= \nu\left\langle \frac{1}{4}\left(\frac{\partial u'_i}{\partial x_j} - \frac{\partial u'_j}{\partial x_i}\right)^2 \right\rangle \\ &= \nu\left\langle S'_{ij}S'_{ij} \right\rangle - \nu\left\langle \frac{\partial u'_j}{\partial x_i}\frac{\partial u'_i}{\partial x_j} \right\rangle \\ &= \nu\left\langle S'_{ij}S'_{ij} \right\rangle - \nu\frac{\partial}{\partial x_i \partial x_j}\left\langle u'_j u'_i \right\rangle \\ &= \nu\left\langle S'_{ij}S'_{ij} \right\rangle - \nu\frac{d^2}{dy^2}\left\langle v'v' \right\rangle \end{aligned}$$

Where statistical independence is used together with the continuity equation of the fluctuating velocity field. Hence in total the following holds

$$\nu \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right\rangle = 2\nu \left\langle S_{ij}' S_{ij}' \right\rangle - \nu \frac{d^2}{dy^2} \left\langle v'v' \right\rangle$$

E Fortran code

All the `Fortran` code that is presented here is implemented in the subroutine called `CLOSUR`. This subroutine calculates the closuremodel.

E.1 Mason & Thompson SGS model

```
C       The distance from the nearest wall
        dist = y(j) - 0.50D0*dy(j)
        if ( j .gt. 32) then
           dist = 1-dist
        endif
C       Delta is the volume of the i,j,k th cell
        Delta=(dx(i)*dy(j)*dz(k))**(1.0/3.0)
        ls = (1.0D0/(Cs*Delta)) + (1.0D0/(Kappa*dist))
        ls = 1.0D0/ls
C       The total viscosity is the sum of the molecular
C       and eddy viscosity
        nu(i,j,k) = (1.0D0/re)  + (ls**2)*2.0D0*SQRT(qq)
```

E.2 Dynamic model

```
C       The alternative tensor PSI is calculated. PSI = -S*4*sqrt(qq)
C       This will be used (in meanxz) to calculate terms used for the
C       the adaptive model
        do mi=1,3
        do mj=1,3
        PSI(i,j,k,mi,mj)= - s(mi,mj)*4.0D0*SQRT(qq)
        end do
        end do
        Delta=(dx(i)*dy(j)*dz(k))**(1.0/3.0)
        if (j .le. 32) then
           tau = (9.0E0*(u1mn(1)-0.0D0)/(re*0.5E0*dy(1))
     &               - (u1mn(2)-0.0D0)/(re*(dy(1)+0.5E0*dy(2))))/8.0E0
           utau=sqrt(tau)

           dist= y(j)-0.5D0*dy(j)
           if (j .le. 15) then
              lsf(i,j,k) =-(1.0D0/mass)*((meanP(i+1,j,k)-
     &     meanP(i-1,j,k))/(dxs(i) + dxs(i-1)))
C        In the log-law layer du/dy=utau/(kappa*y)
           soo2(j)=meanPSI(j,1,2)*(utau/(Kappa*dist))
C        corr is the correction of phi, to prevent discr errors
           visdis=utau/(Kappa*dist)
              if (j .le. 3) then
C        In the viscous sublayer, u+=y+
```

```
                 corr=dist*Kappa*utau*re
                 soo2(j)=meanPSI(j,1,2)*(utau**2)*re
                 visdis=(utau**2)*re
              elseif (j .lt. 8) then
                 corr=((LOG(dist+0.5D0*dy(j))-LOG(dist-0.5D0*dy(j)))
     &              /(dy(j)))*dist
              else
                 corr=1.0D0
              endif
              lss(i,j,k) = (((corr*utau*(utau**2 - lsf(i,j,k)*
     &           (dist)))/(kappa*dist))
     &           - tres1(j) - tres2(i,j,k)+ (1.0D0/re)*meanvis(j)
     &           -(1.0D0/re)*(visdis**2))/
     &           (soo1(j)-soo2(j))
              if (j .gt. 10 ) then
                 pi = 4.0D0*atan(1.0D0)
C       Blending factor is one for j = 11, zero for j = 15
                 factor = (1.0D0/2.0D0)*(1.0D0 +
     &             COS(((j-11.0D0)/4.0D0)*pi))

                 lss(i,j,k) = factor*lss(i,j,k) + (1.0D0 - factor)*
     &         (1.0D0/((1.0D0/(Cs*Delta)) + (1.0D0/(Kappa*dist))))**2
              endif
           elseif (j .gt. 15) then
C       Outside the log-layer, Mason & Thompson wall-damping is used
               lss(i,j,k) = (1.0D0/((1.0D0/(Cs*Delta)) +
     &      (1.0D0/(Kappa*dist))))**2
           endif
        elseif (j .gt. 32) then
C       Symmetry of lengthscale in the wall-normal direction
           lss(i,j,k) = lss(i,ny-j+1,k)
        endif
        lstemp = ABS(lss(i,j,k)*2.0D0*SQRT(qq))
C       Dynamic model is applied after a few time steps, to
C       initialise some values used in the model
        if (n .gt. 2) then
           nu(i,j,k) = (1.0D0/re) + lstemp
        else
           if (j .le. 32) then
              dist= y(j)-0.5D0*dy(j)
           elseif (j .gt. 32) then
              dist= y(ny-j+1)-0.5D0*dy(ny-j+1)
           endif
           nu(i,j,k) = (1.0D0/re) + 2.0D0*SQRT(qq)*(1.0D0/
     &      ((1.0D0/(Cs*Delta)) + (1.0D0/(Kappa*dist))))**2
        endif
```

Furthermore all the mean terms occuring in the dynamic model are calculated in the subroutine called `MEANXZ` . However since this is quite straightforward and lengthy it will be omitted here. In addition, also those mean terms are saved in `mnsXX.dat` at the end of every run, such that they can be used if more than one run is desired.

A brief summary of variables mentioned in the code and how they relate to the model:

Fortran code	Model	Calculated in
PSI(I,J,K,mi,mj)	$\Psi_{mi,mj}^{I,J,K} \equiv -2\lvert\bar{S}\rvert^{I,J,K}\bar{S}_{mi,mj}^{I,J,K}$	CLOSUR
soo2(J)	$\langle\Psi_{12}\rangle^{J}\,\frac{d\langle\bar{u}\rangle}{dy}^{J}$	CLOSUR
visdis(J)	$\frac{d\langle\bar{u}\rangle}{dy}^{J}$	CLOSUR
lsf(I,J,K)	$f^{I,J,K} = -\frac{1}{\rho}\frac{\delta\langle\bar{p}\rangle}{\delta x}^{I,J,K}$	CLOSUR & MEANXZ
tres1(J)	$\left\langle \bar{u}_i' \frac{\partial \bar{u}_i'\bar{u}_j'}{\partial x_j}\right\rangle^{J}$	MEANXZ
tres2(I,J,K)	$\frac{1}{\rho}\left\langle \bar{u}_i' \frac{\partial \bar{p}'}{\partial x_i}\right\rangle^{I,J,K}$	MEANXZ
meanvis(J)	$\left\langle \bar{u}_i' \frac{\partial^2 \bar{u}_i'}{\partial x_j \partial x_j}\right\rangle^{J}$	MEANXZ
soo1(J)	$\left\langle \frac{\partial \Psi_{ij}'}{\partial x_j}\bar{u}_i'\right\rangle^{J}$	MEANXZ

All global variables, which are calculated in MEANXZ, can be called by including var/dynamic.