Report on different large eddy simulation models.
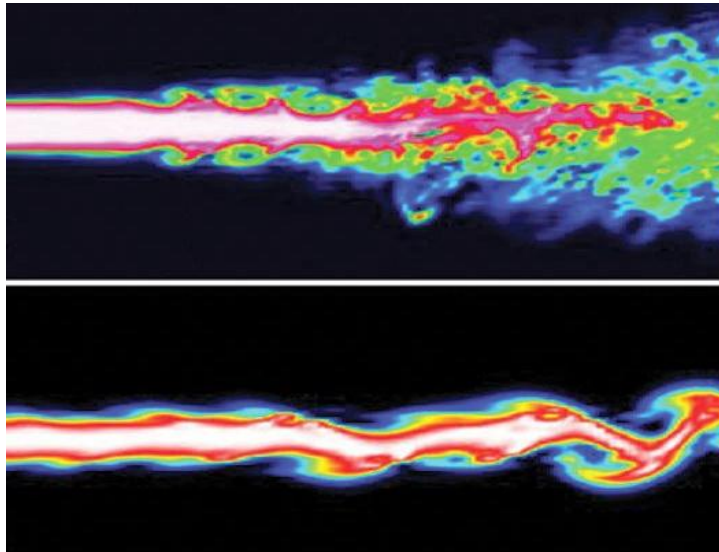
Bachelor thesis Applied Mathematics

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Abstract

This thesis looks at the theory behind different large eddy simulation models and aims for a basic understanding in the topic. The aim of large eddy simulations is to model a turbulence flow by preserving most of its properties, like the effects from smaller eddies on the larger eddies, but without the full cost of a direct numerical simulation (DNS). The models discussed in this thesis are the approximate deconvolution procedure (ADP), the scale residual method (SRM) and the eddy viscosity method (EVM). In the research of this thesis a channel flow is simulated by the Clark model and qr-model which are examples of the ADP and EVM models, respectively. These results are tested versus the DNS data and the theoretical frame provided by the law of the wall. Further there is also a custom made large eddy simulation model for this thesis, which results are also included in the research. It turns out that the Clark model, qr-model and the custom model all comply with the wall of the law and the DNS data.

Contents

1: Introduction on large eddy simulations

The modeling of the flow of a fluid is an active field of research, with many applications. A group of important models are the Navier-Stokes equations, which have been around since 1822. However, there have still been found only a few algebraic solutions to some specific cases, but not yet a global exact solution, which makes most models impossible to solve by hand. However, computers have made it possible to compute these models by using numerical mathematical methods. This does not mean that these methods are easily to use. Most of these methods are costly and take a lot of time to compute, even for super computers. That is why applied mathematicians try to simplify these problems, without losing much of the solution.

To decrease the costs of numerically solving the Navier-Stokes equations we use large eddy simulations. The global idea of a large eddy simulation is that we try to evaluate the global flow of a fluid, without modeling the smaller flows. This does not mean that we negate the effect of the smaller flows, since these smaller flows may lead to big effects in the fluid.

In this paper we will test some large eddy simulation models and give a detailed description of some of these models. This first chapter is dedicated to some principal aspects of fluid dynamics like the Navier-Stokes equation and some basic mathematical aspects like filters and Fourier series. These basic aspects will give a better understanding of the large eddy simulation models which we will discuss in Chapter 2. The third chapter is dedicated to a flow in a channel which we use to test some models.

1.1   Navier-Stokes equations

The Navier Stokes equations describe the motion of a fluid. As mentioned before, the equations have been around since 1822, when Claude-Louis Navier first expanded the Euler equations by introducing molecular forces. Twenty years later, these molecular forces were linked to viscous forces by Adhémar Jean Claude Barréde Saint-Venant. Another two years later George Gabriel Stokes expanded Saint-Venants model, which led to the current Navier-Stokes equation.

1.1.1 Restrictions and assumptions

In this paper the following restrictions and assumptions are laid on the fluid which will be modeled.

- It is assumed that a flow can be modeled by a continuous model, which is plausible on macro-scale but is doubtful on micro-scale. On micro-scale other effects may be involved like the interaction between specific molecules, while these effects on macro-scale are irrelevant small.

- The fluid should be incompressible, which means that the density ρ is constant over time and space.

- The fluid is of a constant temperature, since a difference in temperature may lead to a fluctuation in the density or other terms.

- The Navier-Stokes equations does not apply to non Newtonian fluids. Examples of a non Newtonian fluid is ketchup, which clearly flows different then water, which is a Newtonian fluid. The Navier-Stokes equation only applies for Newtonian fluids and that is why we assume that the fluid is Newtonian.

1.1.2 Derivation of the Navier-Stokes equation

In this section there will be a brief derivation of the Navier-Stokes equation. First we start with the equation for the conservation of mass. Take a arbitrary volume V. There will not appear or disappear any mass in V other than which flows through its boundary S. So the only difference of the mass of V is determined by the flow in and out of the boundary. This will lead to,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_V \rho \, \mathrm{d}\mathbf{x} = -\int_S (\rho \mathbf{u}) \cdot \mathbf{n} \, \mathrm{d}S. \tag{1.1}$$

where $\mathbf{n}$ denotes the normal unit vector to S. The right-hand side can be written as a volume with the help of the divergence theorem that states that the outward flux on a closed surface can be expressed in the gradient on the whole domain. Applying this theorem to Equation (1.1) results into,

$$\int_V \rho_t + \nabla \cdot (\rho \mathbf{u}) \, \mathrm{d}\mathbf{x} = 0.$$

Since the flow was assumed to be continuous in the previous section it follows that,

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0$$

The next step follows from another restriction that was also stated in the previous section. Since the flow is assumed to be incompressible it follows that the density ρ does not change over time and space, so $\rho(\mathbf{x}, t) \equiv \rho_0$. Thus, the first term of the previous equation disappears, since the derivative of a constant term is zero. The density cannot be zero and so it is possible to divide ρ out of the equation. This will lead to the incompressibility condition,

$$\nabla \cdot \mathbf{u} = 0. \tag{1.2}$$

Next the Navier-Stokes equation will be derived from Newtons second law, *the force on a particle equals its mass times its acceleration*. This is also called the momentum equation. The acceleration

of a particle is given by the derivative to time of $\mathbf{u}(\mathbf{x}(t), t)$. The velocity of a particle on $t + \Delta t$ is given by $\mathbf{u}(\mathbf{x} + \Delta t \mathbf{u}(\mathbf{x}, t), t + \Delta t)$. This makes the acceleration $\mathbf{a}$,

$$\mathbf{a} = \lim_{\Delta t \to 0} \frac{\mathbf{u}(\mathbf{x} + \Delta t \mathbf{u}(\mathbf{x}, t), t + \Delta t) - \mathbf{u}(\mathbf{x}, t)}{\Delta t} = \mathbf{u}_t + \sum_{j=1}^{d} u_j \frac{\partial u_i}{\partial x_j} = \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u},$$

with d the dimension ($d = 3$ in $\mathbf{R}^3$). Using Newtons Second law the momentum of the earlier defined volume V is given by:

$$\int_V \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) \, \mathrm{d}\mathbf{x}$$

The momentum must be balanced with other forces, these are the external body forces ($\mathbf{f}$) and contact forces ($\mathbf{t}(\mathbf{s})$). Since the body forces are defined on the volume V and contact forces only on the boundary S the force balance is given by,

$$\int_V \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) \, \mathrm{d}\mathbf{x} = \int_V \mathbf{f} \, \mathrm{d}\mathbf{x} + \int_S \mathbf{t}(\mathbf{s}) \, \mathrm{d}S. \tag{1.3}$$

Examples of external forces are gravity and electromagnetic forces. These forces can not be defined anymore specific since they depend on the modeled situation. However, there can be said something about the internal forces $\mathbf{t}$. These are mostly determined by pressure and viscous forces and they are defined on the surface S of V since they are contact forces. From an idea of Cauchy it follows that $\mathbf{t}$ only depends on the normal vector $\mathbf{n}$ of the surface S in the following way:

$$\mathbf{t}(\mathbf{n}) = \boldsymbol{\sigma} \cdot \mathbf{n}, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{x}, t). \tag{1.4}$$

Where $\boldsymbol{\sigma}$ is the stress tensor. This stress tensor is a $d \times d$ matrix which represents both the the pressure forces and the viscous forces. In an incompressible fluid we have,

$$\boldsymbol{\sigma} = -\mathbf{p}I + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \tag{1.5}$$

With μ the viscosity and $\frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ the strain rate tensor $S(\mathbf{u})$. From Equation (1.4) and Equation (1.5) it follows that Equation (1.3) can be written as:

$$\int_V \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) \, \mathrm{d}\mathbf{x} = \int_V \mathbf{f} \, \mathrm{d}\mathbf{x} + \int_S \mathbf{n} \cdot \boldsymbol{\sigma} \, \mathrm{d}S = \int_V \mathbf{f} - \nabla \mathbf{p} + \mu \Delta \mathbf{u} \, \mathrm{d}V$$

Since the volume V is arbitrary and the integrand is assumed to be continuous we arrive at,

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla \mathbf{p}}{\rho} - \frac{\mu}{\rho} \Delta \mathbf{u} = \frac{1}{\rho} \mathbf{f} \tag{1.6}$$

Equation (1.6) can be simplified by redefining $\frac{\mathbf{p}}{\rho}$ by $\mathbf{p}$ and $\frac{\mathbf{f}}{\rho}$ by $\mathbf{f}$. The term $\frac{\mu}{\rho}$ is called the kinematic viscosity ν. This lead with Equations (1.2) and (1.6) to the incompressible Navier-Stokes equation:

$$\begin{aligned} \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \mathbf{p} - \nu \Delta \mathbf{u} &= \mathbf{f} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \tag{1.7}$$

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1.1.3 Scaled Navier-Stokes equation

The Navier-Stokes Equation (1.7) can be scaled in such a way that all variables are dimensionless. The dimensions of the variables are $[\mathbf{u}] = T^{-1}L$, $[\mathbf{x}] = L$ and $[\mathbf{p}] = T^{-2}M$. A logical choice for scaling the space and time variables would be,

$$\hat{\mathbf{v}} = \frac{\mathbf{v}}{V_0}, \qquad \hat{\mathbf{x}} = \frac{\mathbf{x}}{L_0} \tag{1.8}$$

Here L_0 is the characteristic length of the largest wavelength in the flow and V_0 is the initial velocity. The dimension of the density is given by $[\rho] = L^{-3}M$. It can be seen that the pressure, the time, the density and the gradient can all be scaled with only L_0 and V_0 in the following way,

$$\hat{\mathbf{p}} = \frac{\mathbf{p}}{\rho_0 V_0^2}, \qquad \hat{t} = \frac{tV_0}{L_0}, \qquad \hat{\rho} = \frac{\rho}{\rho_0}, \qquad \hat{\nabla} = L_0 \nabla. \tag{1.9}$$

By substituting Equation (1.8) and Equation (1.9) in the Navier Stokes equation without external forcing ($\mathbf{f} = 0$) we get the scaled Navier-Stokes equation. After some rewriting the scaled Navier-Stokes equation is given by,

$$\hat{\mathbf{u}}_{\hat{t}} + \hat{\mathbf{u}} \cdot \hat{\nabla}\hat{\mathbf{u}} = -\hat{\nabla}\hat{p} + \frac{\nu}{L_0 V_0}\hat{\Delta}\hat{\mathbf{u}}.$$

All variables are now dimensionless and the only number involved in this equation is

$$Re = \frac{L_0 V_0}{\nu},$$

which is called the Reynolds number. The Reynolds number of a flow shows some properties of flow, since flows with similar Reynolds numbers tend to have similar properties. An interesting example of the use of the Reynolds number is for testing prototypes of planes. Since the length of the prototype is often much smaller than the real product, the velocity and viscosity can be adjusted to make it still possible to do tests which will give similar results as the real plane would. The Reynolds number can also predict if a model could have certain problems with simulations.

1.2 Fourier space

To illustrate properties of the Navier-Stokes equation it is useful to use the Fourier transform of the Navier-Stokes equation. The Fourier transform of a function is expressed as the infinite sum of harmonic components, which are expressed in time t and frequencies ω, or like in the case of Navier-Stokes equation in wavenumber κ. The Fourier transform exist for every piecewise continuous and absolutely integrable function and is given by,

$$\mathbf{f}(t) = \sum_{\kappa=1}^{\infty} \widehat{\mathbf{f}}_\kappa e^{i\kappa t},$$

where $\widehat{\mathbf{f}}_\kappa$ is called the Fourier transform and is given by,

$$\widehat{\mathbf{f}}_\kappa = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^d} \mathbf{f}(t) e^{-i\kappa\mathbf{x}} \, \mathrm{d}\mathbf{x}.$$

From now on we will write $\widehat{\mathbf{f}}(t)$ when we take the Fourier transform of the function $\mathbf{f}(t)$.

1.2.1   The frequency spectrum of the NS-Equation

The Fourier transform of the Navier-Stokes equation exists since every flow is piecewise continuous and absolutely integrable. This is true because it was already assumed that the fluid could be modeled by a continuous model and the fluid is absolutely integrable since we assume that $\mathbf{u}$ will be bounded. Here a derivation of the Fourier transform of the Navier-Stokes equation will be given,

$$\widehat{\mathbf{u}_t} + \widehat{\mathbf{u} \cdot \nabla \mathbf{u}} + \widehat{\nabla \mathbf{p}} - \nu \widehat{\Delta \mathbf{u}} = \widehat{\mathbf{f}}_\kappa$$

From the definition of the Fourier transform we know that the time derivative commutes with integration, so $\widehat{\mathbf{u}_t} = \widehat{\mathbf{u}}_t$. Integration by parts shows that,

$$
\begin{aligned}
\widehat{\nabla \mathbf{f}(x)} &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^d} \nabla \mathbf{f}(x) e^{-i\kappa \mathbf{x}} \, \mathrm{d}\mathbf{x} \\
&= i\kappa \frac{1}{(2\pi)^3} \int_{\mathbb{R}^d} \mathbf{f}(x) e^{-i\kappa \mathbf{x}} \, \mathrm{d}\mathbf{x} \\
&= i\kappa \widehat{\mathbf{f}},
\end{aligned}
$$

as long as the boundary terms vanishes, which happens for periodic boundary conditions e.g.. For the Laplacian the same follows, so $\widehat{\Delta \mathbf{f}} = -\kappa^2 \widehat{\mathbf{f}}$. We now have,

$$\widehat{\mathbf{u}}_t + \widehat{\mathbf{u} \cdot \nabla \mathbf{u}} + i\kappa \widehat{\mathbf{p}} + \nu \kappa^2 \widehat{\mathbf{u}} = \widehat{\mathbf{f}}$$

The remaining part is a lot more work and not very important for this paper. We will note $\widehat{\mathbf{u} \cdot \nabla \mathbf{u}}$ as $P(\mathbf{u} \cdot \nabla \mathbf{u})$. A full formulation in the spectral space of the Navier-Stokes equation can be found in *Large Eddy Simulation for Incompressible Flows* from *P. Sagaut.* [3]

1.2.2   Convolution Product

An important property of the Fourier transpose arises in the convolution product. For two functions f and g the convolution is given by,

$$(f \star g)(\mathbf{x}) := \int_{\mathbb{R}^d} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y}) \, \mathrm{d}\mathbf{y}.$$

The convolution product has the following property,

$$
\begin{aligned}
\widehat{(f \star g)} &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y}) \, \mathrm{d}\mathbf{y} \right) e^{-i\kappa \mathbf{x}} \, \mathrm{d}\mathbf{x} \\
&= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} f(\mathbf{x} - \mathbf{y}) e^{-i\kappa \mathbf{x}} \, \mathrm{d}\mathbf{x} \right) g(\mathbf{y}) \, \mathrm{d}\mathbf{y} \\
&= \frac{1}{(2\pi)^3} \widehat{f} \int_{\mathbb{R}^d} g(\mathbf{y}) e^{-i\kappa \mathbf{y}} \, \mathrm{d}\mathbf{y} \\
&= \widehat{f} \, \widehat{g}
\end{aligned}
$$

The third equality follows when we substitute $\mathbf{x} - \mathbf{y}$ for another variable. We see that the Fourier transform of the convolution is the same as the product of the individual Fourier transforms. This property will be used for filters which will be discussed next.

1.3 Filters

Filters are the key to large eddy simulation, so to understand large eddy simulations we first need to understand filters.

1.3.1 Properties

Basically a filter suppresses high frequencies in the spectral space. We apply a filter G to a function f with the convolution product as defined in Section 1.2.2. So if we want to filter f we get $(G \star f)(x)$ in the physical space and $\hat{G}\hat{f}$ in the spectral space. We will note $(G \star f)(x)$ as $G(f)$, to emphasize that we filter the function f. There are a lot of different filters. The filters we are interested in have the following properties:

- *Conservation of constants.*
    We have that for any constant a it follows that $G(a) = a$. Note that from this property it follows that $\displaystyle\int_{\mathbb{R}^d} G(\mathbf{x} - \mathbf{y})\,\mathrm{d}^d\mathbf{y} = 1$

- *Linearity.*
    For any two functions f and g we have $G(f + g) = G(f) + G(g)$.

- *Commutation with derivation.*
    If we take the derivative of f we get $\dfrac{\mathrm{d}G(f)}{\mathrm{d}s} = G\!\left(\dfrac{\mathrm{d}f}{\mathrm{d}s}\right)$.

1.3.2 Commutator

We introduce a new notation for the third property, the commutator. The commutator is given by,

$$\big[f, g\big](x) = f \circ g(x) - g \circ f(x) = f(g(x)) - g(f(x))$$

So the third property noted in Section 1.3.1 can be written as,

$$\left[G\star, \frac{\mathrm{d}}{\mathrm{d}s}\right] = 0$$

1.3.3 Physical and Spectral space

The following filters are the mostly used ones. They are plotted in the physical and the spectral space. Note that the filters are all plotted for $\xi = 0$, which could give plots in the spectral space with negative wave numbers. Since negative wave numbers have no meaning they can be ignored. They are still shown here since a different value for ξ shifts the figure.

1.3.3.1 Top hat filter

We start with the top hat filter, which is also called the box filter or the moving averaged. The formula in the physical space is given by,

$$G(x - \xi) = \begin{cases} 1/\bar{\Delta} & \text{if } |x - \xi| \leq \bar{\Delta}/2 \\ 0 & \text{otherwise} \end{cases}$$

and in the spectral space by,

$$\hat{G}(\kappa) = \frac{sin(\kappa\Delta/2)}{\kappa\Delta/2}$$

Here $\bar{\Delta}$ is the radius of the spatial filter. The next plots of the top hat filter are the physical space and the spectral space, both with $\bar{\Delta} = 1$.
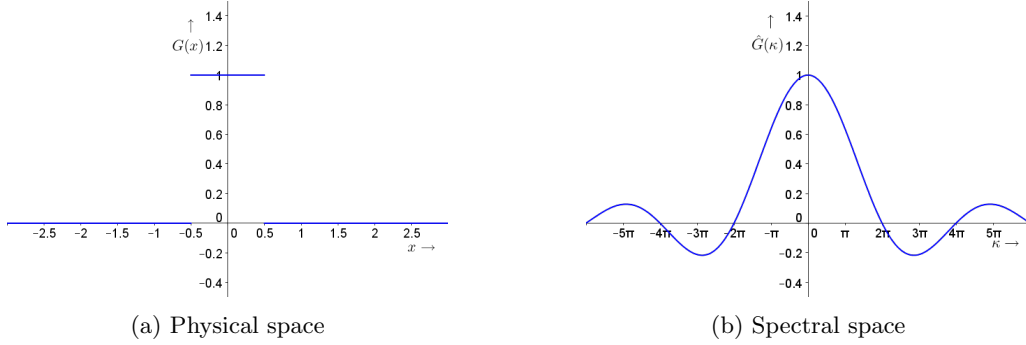

(a) Physical space   (b) Spectral space

Figure 1.1: The top hat filter

We see that the top hat filter is a positive filter, since $G(x - \xi) \geq 0$ for every x. Futher we see that G is local in the physical space, which means that $G(\mathbf{x})$ is nonzero in a finite interval. It can be seen that $\hat{G}(\kappa)$ is non local.

1.3.3.2   Gaussian filter

Another popular filter is the Gaussian filter, which is given in the physical space by,

$$G(x - \xi) = \left(\frac{\gamma}{\pi\bar{\Delta}^2}\right)^{1/2} e^{\frac{-\gamma|x-\xi|^2}{\bar{\Delta}^2}}$$

And in the spectral space by,

$$\hat{G}(\kappa) = e^{\frac{-\bar{\Delta}^2\kappa^2}{4\gamma}}$$

The interesting thing about this filter is that the function is a Gaussian function in both the physical and spectral space. Gaussian functions are functions of the form $f(x) = ae^{-\left(\frac{x-b}{c}\right)^2}$, where a, b and c are all real constants. Properties of Gaussian functions are that they are symmetric and positive and $\int_{-\infty}^{\infty} ae^{-\left(\frac{x-b}{c}\right)^2} dx = ac\sqrt{\pi}$. So a Gaussian function is an Gaussian filter if $ac = \frac{1}{\sqrt{\pi}}$, which indeed is the case for $a = \frac{1}{\sqrt{\pi}\bar{\Delta}}$ and $c = \bar{\Delta}$. The plots of the physical space and the spectral space are given by,
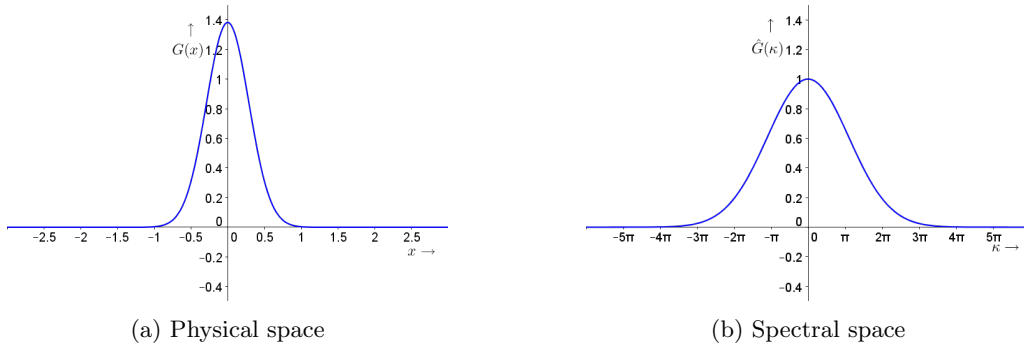
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(a) Physical space

(b) Spectral space

Figure 1.2: The Gaussian filter

We see in both figures the recognizable form of Gaussian functions. Just like the top hat filter is the Gaussian filter positive in the physical space, but this time also in the spectral space. However, the Gaussian function is not local, which requires a cut off for implementation in computations.

1.3.3.3 Sharp cutoff filter

The sharp cutoff filter is similar to the top hat filter, but this time we look at specific wavenumbers in the spectral plane, instead of values of the physical plane.

$$G(x - \xi) = \frac{sin(\pi/\bar{\Delta}(x - \xi))}{\pi/\bar{\Delta}(x - \xi)}$$

$$\hat{G}(\kappa) = \left\{ \begin{array}{ll} 1 & \text{if } |\kappa| \leq \pi/\bar{\Delta} \\ 0 & \text{otherwise} \end{array} \right.$$

(a) Physical space

(b) Spectral space

Figure 1.3: The sharp cutoff filter
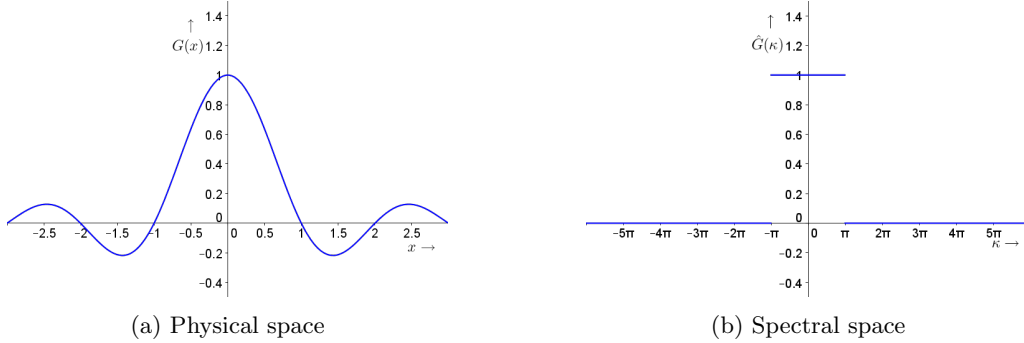
We see that the plots of the sharp cutoff filter and the top hat filter are very similar, but with the physical and spectral space reversed. Of these three filters the sharp cutoff filter is the only one with the property $\hat{G}(\hat{G}(\hat{G}...))) = \hat{G}$, so it is idempotent in the spectral space. It is also the only of these three which is local in the spectrum space.

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1.4 Filtered Navier Stokes equation

We will now combine filters with the Navier-Stokes equation. If we apply a filter G to a function f we will remain with a filtered function $\overline{f}$ and the residue would be $\tilde{f}$. So we have,

$$\begin{aligned} G(f) &= \overline{f} \\ f &= \overline{f} + \tilde{f} \end{aligned} \tag{1.10}$$

With the previous stated properties in Section 1.3.1, a filter would have the following results on the Navier-Stokes equation (Equation (1.7)),

$$\begin{aligned} G(\mathbf{u}_t) + G(\mathbf{u} \cdot \nabla \mathbf{u}) + G(\nabla \mathbf{p}) - G(\nu \Delta \mathbf{u}) &= G(\mathbf{f}) \\ \overline{\mathbf{u}}_t + G(\mathbf{u} \cdot \nabla \mathbf{u}) + \nabla \overline{\mathbf{p}} - \nu \Delta \overline{\mathbf{u}} &= \overline{\mathbf{f}} \end{aligned}$$

The non linear term can not be filtered as simple as the other terms. So we will look more closely at this term. First we rewrite the non linear term with the second line of Equation (1.10).

$$\begin{aligned} G(\mathbf{u} \cdot \nabla \mathbf{u}) &= G((\overline{\mathbf{u}} + \tilde{\mathbf{u}}) \cdot \nabla (\overline{\mathbf{u}} + \tilde{\mathbf{u}})) \\ &= G(\overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}}) + G(\overline{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}}) + G(\tilde{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}}) + G(\tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}}) \end{aligned} \tag{1.11}$$

From Equation (1.11) we get the following terms,

- The cross-stress tensor C, which are the stresses between the main-grid and the sub-grid of the filter.

$$C = G(\overline{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}}) + G(\tilde{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}})$$

- The Reynold sub-grid tensor R, which are all terms determined by only the sub-grid.

$$R = G(\tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}})$$

We suppose that since these terms fully exists from sub-grid components that these terms will be filtered out completely.

- The Leonard tensor L, which are all terms determined by only the main-grid.

$$L = G(\overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}})$$

Modeling R, C and L is hard, that is why most models try to find smart ways around these. When we discuss some large eddy simulation models we will talk about ways to model these term, but for now the following definition of the filtered Navier-Stokes equation is sufficient.

$$\overline{\mathbf{u}}_t + C + L + \nabla \overline{\mathbf{p}} - \nu \Delta \overline{\mathbf{u}} = \overline{\mathbf{f}} \tag{1.12}$$

1.5 Energy equation in the spectrum

In this section the Navier-Stokes equation is taken in such a way that the pressures does not contribute in the equation, this is further explained in *Estimate for the energy cascade in three-dimensional flows* by *Dr. C. Foias and O.P. Manley and Dr. R.M.S.Roas and Dr. R.Temam* and earlier works in that series. [2]. From this version of the Navier-Stokes equation is derived the energy equation by taking the inner product with $\mathbf{u}(t)$, with the inner product defined by $(\mathbf{u}, \mathbf{v}) = \int_V \mathbf{u} \cdot \mathbf{v} \, d\mathbf{x}$.

$$(\mathbf{u}_t \cdot \mathbf{u}) + (\mathbf{u} \cdot \nabla \mathbf{u} \cdot \mathbf{u}) - \nu(\Delta \mathbf{u} \cdot \mathbf{u}) = (\mathbf{u} \cdot \mathbf{f})$$

When we take a look at this equation in the frequency spectrum we see that,

$$\frac{1}{2}\frac{d}{dt}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 + \nu|\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 = (\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) + e_{\kappa_1} - e_{\kappa_2}, \tag{1.13}$$

This is explained in Appendix A. Instead of looking at a specific time, we now look at the average on the whole time domain. Therefor we introduce the following notation

$$\langle \phi \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T \phi(\mathbf{u}(t)) \, dt.$$

For the limit to exists we need $\phi(\mathbf{u})$ to be uniformly bounded. Without loss of generality we can state that $|\mathbf{u}_{\kappa_1,\kappa_2}|$, $|\mathbf{u}_{\kappa_1,\kappa_2}|$ and $|\nabla \mathbf{u}_{\kappa_1,\kappa_2}|$ are all uniformly bounded. Taking the time average of Equation (1.13) results in,

$$\langle \frac{1}{2}\frac{d}{dt}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle + \langle \nu|\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle = \langle (\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) \rangle + \langle e_{\kappa_1} \rangle - \langle e_{\kappa_2} \rangle \tag{1.14}$$

We note that the first term is zero because,

$$\begin{aligned}
\langle \frac{1}{2}\frac{d}{dt}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle &= \lim_{T\to\infty} \frac{1}{T} \int_0^T \frac{1}{2}\frac{d}{dt}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 \, dt \\
&= \lim_{T\to\infty} \frac{1}{2T}\left[|\mathbf{u}_{\kappa_1,\kappa_2}(T)|^2 - |\mathbf{u}_{\kappa_1,\kappa_2}(0)|^2 \right] = 0.
\end{aligned} \tag{1.15}$$

So we are left with

$$\langle \nu|\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle = \langle (\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) \rangle + \langle e_{\kappa_1} \rangle - \langle e_{\kappa_2} \rangle$$

We now look at some specific wave numbers. We introduce $\kappa_\mathbf{f}$ as the maximum wavenumber where the external forces has effect, so for $\kappa_\mathbf{f} < \kappa_1 < \kappa_2$ we have $(\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) = 0$. By using these wave numbers and Equation (1.15) we can rewrite Equation (1.14) and state that:

$$\nu\langle |\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle = \langle e_{\kappa_1} \rangle - \langle e_{\kappa_2} \rangle \tag{1.16}$$

We suppose $\langle e_\infty \rangle = 0$ and so we can state the following,

$$\nu\langle |\nabla \mathbf{u}_{\kappa_1,\infty}|^2 \rangle \leq \langle e_{\kappa_1} \rangle \tag{1.17}$$

From Equation (1.17) we know that $\langle e_{\kappa_1} \rangle \geq 0$ for every $\kappa > \kappa_\mathbf{f}$, since the left-hand side consists of a positive scalar and a square of a real value, so Equation (1.17) is always positive. Since

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$\kappa_2 > \kappa_1 > \kappa_{\kappa_f}$ it follows from Equation (1.16) that $\langle e_{\kappa_2} \rangle \leq \langle e_\kappa \rangle$, so we know that $\langle e_\kappa \rangle$ is positive and monotonic decreasing for every $\kappa \geq \kappa_f$. This can be seen in Figure 1.4.
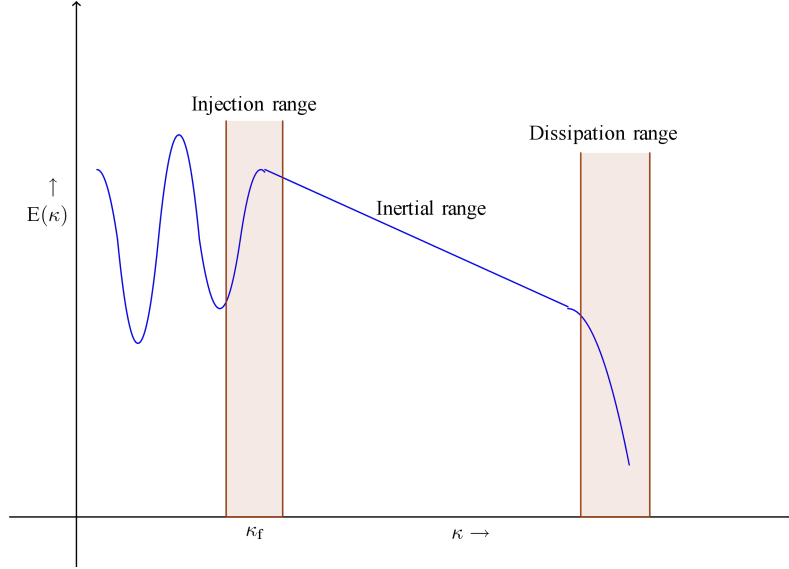

Figure 1.4: Energy of the flow

1.5.1 Notation and specific wave numbers

Before we look any further at the energy equation we first introduce some notation, as in *Turbulence* by *U. Frisch.* [6]

· The mean energy dissipation.
$$\epsilon \equiv \nu \langle |\nabla \mathbf{u}|^2 \rangle$$

· The average kinetic energy
$$E \equiv \frac{1}{2} \langle |\mathbf{u}|^2 \rangle$$

There is also one important wavenumber worth mentioning which is the Taylor wavenumber. The Taylor wavenumber is defined by $\kappa_\tau = \left(\frac{\langle \|\nabla \mathbf{u}\|^2 \rangle}{\langle |\mathbf{u}|^2 \rangle} \right)^{\frac{1}{2}}$.

1.5.2 Behavior

We will now try to determine some bounds and the behavior of the energy transport ($\langle \mathbf{e}_\kappa(\mathbf{u}) \rangle$) over the wave numbers $\kappa_2 > \kappa_1 > \kappa_{\kappa_f}$, which will also explain more about Figure 1.4. But first the following bound is assumed:

$$(\langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle - \langle \mathbf{e}_{\kappa_2}(\mathbf{u}) \rangle = \nu \langle |\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle \leq \nu \kappa_2^2 \langle |\mathbf{u}_{\kappa_1,\kappa_2}|^2 \rangle \tag{1.18}$$

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The first part is Equation (1.16) and for the second part follows from the next steps.

$$|\nabla \mathbf{u}|^2 = \int_\Omega (\nabla \mathbf{u}, \nabla \mathbf{u}) \mathrm{d}\mathbf{x}$$

Which can be rewritten as follows,

$$\int_\Omega (\nabla \mathbf{u}, \nabla \mathbf{u}) \mathrm{d}\mathbf{x} = - \int_\Omega (\mathbf{u}, \Delta \mathbf{u}) \mathrm{d}\mathbf{x} \leq \lambda |\mathbf{u}|$$

Where λ is the largest eigenvalue of the Laplacian, which was stated in Section 1.2.1 to be κ^2. Since $\mathbf{u}_{\kappa_1, \kappa_2}$ is only defined for κ in $[\kappa_1, \kappa_2]$ it follows that,

$$|\nabla \mathbf{u}_{\kappa_1, \kappa_2}| \leq \kappa_2^2 |\mathbf{u}_{\kappa_1, \kappa_2}|$$

This will also be true when we take the time average which explains the second equal sign in Equation (1.18). We will now pick up Equation (1.18) again to make a further approximation for the upper bound.

$$\nu \langle |\nabla \mathbf{u}_{\kappa_1, \kappa_2}|^2 \rangle \leq \nu \kappa_2^2 \langle |\mathbf{u}_{\kappa_1, \kappa_2}|^2 \rangle \leq 2\nu \kappa_2^2 E \leq \left(\frac{\kappa_2}{\kappa_\tau}\right)^2 \epsilon \tag{1.19}$$

Where E is the average kinetic energy and ϵ is the average energy, both as defined in *Turbulence* by *U. Frisch* . [6]. On the other hand we have from Equation (1.17),

$$
\begin{aligned}
\langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle \quad &\geq \quad \nu \langle |\nabla \mathbf{u}_{\kappa_1, \infty}|^2 \rangle \\
&= \quad \nu \Big(\langle |\nabla \mathbf{u}_{\kappa_0, \kappa_1}|^2 \rangle - \langle |\nabla \mathbf{u}_{\kappa_0, \kappa_1}|^2 \rangle + \langle |\nabla \mathbf{u}_{\kappa_1, \infty}|^2 \rangle \Big) \\
&= \quad \epsilon - \nu \langle |\nabla \mathbf{u}_{\kappa_0, \kappa_1}|^2 \rangle \\
&= \quad \left(1 - \left(\tfrac{\kappa_1}{\kappa_\tau}\right)^2 \right) \epsilon
\end{aligned}
$$

Equation (1.19) is equivalent to,

$$\left(1 - \left(\frac{\kappa_1}{\kappa_\tau}\right)^2 \right) \epsilon \leq \langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle \quad \Longleftrightarrow \quad \epsilon \leq \left(1 - \left(\frac{\kappa_1}{\kappa_\tau}\right)^2 \right)^{-1} \langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle \tag{1.20}$$

If we put Equation (1.18), Equation (1.19) and Equation (1.20) together it follows that,

$$0 \leq (\langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle - \langle \mathbf{e}_{\kappa_2}(\mathbf{u}) \rangle) \leq \left(\frac{\kappa_2}{\kappa_\tau}\right)^2 \left(1 - \left(\frac{\kappa_1}{\kappa_\tau}\right)^2 \right)^{-1} \langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle$$

or

$$0 \leq 1 - \frac{\langle \mathbf{e}_{\kappa_2}(\mathbf{u}) \rangle}{\langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle} \leq \left(\frac{\kappa_2}{\kappa_\tau}\right)^2 \left(1 - \left(\frac{\kappa_1}{\kappa_\tau}\right)^2 \right)^{-1} = \frac{\kappa_2^2}{\kappa_\tau^2 - \kappa_1^2} \tag{1.21}$$

We suppose that $\kappa_\tau \gg \kappa_2$, so we get that the right-hand side will go to zero, which means that $\langle \mathbf{e}_{\kappa_2}(\mathbf{u}) \rangle$ and $\langle \mathbf{e}_{\kappa_1}(\mathbf{u}) \rangle$ are almost equal. In other words, we have stated that the energy over the inertial wavenumber between κ_1 and κ_2 does not change much for $\kappa_f \leq \kappa_1 < \kappa_2 \ll \kappa_\tau$. This process is called energy cascade. [2] We know from Equation (1.21) that the energy over the inertial is no

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longer dependent of ν and only depends on the wave numbers κ and the energy dissipation ϵ. The dimensions of the wavenumber and average energy are,

$$
\begin{array}{rcl}
[\kappa] & = & L^{-1} \\
[\epsilon] & = & L^2 T^{-3}
\end{array}
$$

We know that $E = C\epsilon^a \kappa^b$, with C an dimensionless constant, which experimental value lies around 1.5. From dimension analysis we get,

$$
E = C\epsilon^{\frac{2}{3}} \kappa^{-\frac{5}{3}}
$$

Which is the function for the energy cascade for the inertial range and which explains the slope in Figure 1.4.

2: Different large eddy simulation models

Subject of this chapter are different large eddy simulation models. Some of these models will return in the research part in Chapter 3.

2.1 Approximate Deconvolution Procedure

The first large eddy simulation discussed here is the approximate deconvolution procedure. The theory was made by professor S. Stolz and professor N.A. Nikolaus and the idea is that an inverse of a filter is used to approximate the effects on the sub-grid. In this section there first will be an explanation of the theory of the approximate deconvolution procedure and later as an example the Clark model will be discussed.

2.1.1 The theory

First we introduce a shorter notation for the Navier-Stokes Equation (1.7) without external force terms $\mathbf{f}$.

$$
\begin{array}{rcl}
\mathbf{u} \cdot \nabla \mathbf{u} + \nabla \mathbf{p} - \nu \Delta \mathbf{u} & = & \mathcal{NS}(\mathbf{u}) \\
\mathbf{u}_t + \mathcal{NS}(\mathbf{u}) & = & 0
\end{array}
$$

The filtered Navier-Stokes Equation (1.11) will become,

$$
\begin{array}{rcl}
G(\mathbf{u}_t) + G(\mathcal{NS}(\mathbf{u})) & = & 0 \\
& \Longleftrightarrow & \\
G(\mathbf{u})_t + G(\mathcal{NS}(\mathbf{u})) & = & \mathcal{NS}(G(\mathbf{u})) - \mathcal{NS}(G(\mathbf{u})) \\
& \Longleftrightarrow & \\
G(\mathbf{u})_t + \mathcal{NS}(G(\mathbf{u})) & = & \mathcal{NS}(G(\mathbf{u})) - G(\mathcal{NS})(\mathbf{u})) \\
& = & -[\mathcal{NS}, G](\mathbf{u})
\end{array}
\tag{2.1}
$$

where $[\dots]$ is the commutator as defined in Section 1.3.2. The left-hand side is expressed in $G(\mathbf{u})$, or in other words in terms on the main-grid, while the right-hand side still has components on

sub-grid. Since large eddy simulation models only does computations on the main-grid this could lead to problems. The approximate deconvolution procedure solves this problem by making the following approximation,

$$\mathbf{u} \approx \mathbf{u}_{app} \equiv G^{-1}(G(\mathbf{u}))$$

This would give a perfect result if the inverse would actual exist. However, the inverse of a filter can not exist since filtering is not a bijective operation. If the two functions f and g with $f = \hat{f} + \tilde{f}$, $g = \hat{f} + 2\tilde{f}$ and $f \neq g$, then $G(g) = \hat{f} = G(f)$. So G is not injective. It is still possible to make a kind of approximation to the inverse (G_l^{-1}). So we can rewrite Equation (2.1) as,

$$G(\mathbf{u})_t + \mathcal{NS}(G(\mathbf{u})) = -[\mathcal{NS}, G](G_l^{-1}G(\mathbf{u})) \tag{2.2}$$

By subtracting Equation (2.2) from (2.1) it is possible to get an approximation for the sub-grid term,

$$[\mathcal{NS}, G](\mathbf{u}) \approx [\mathcal{NS}, G](G_l^{-1}G(\mathbf{u}))$$

which is fully expressed in terms of the main-grid. We can now go back to the first line of Equation (2.1) and model the filtered Navier-Stokes equation by the approximate deconvolution procedure as,

$$G(\mathbf{u}_t) + G(\mathcal{NS}(G_l^{-1}(G(\mathbf{u})))) = 0$$

where the efficiency is determined by the quality of the estimation of G^{-1}.

2.1.2 The Clark model

The Clark model is an example of an approximate deconvolution method which uses a Taylor expansion of the Gaussian filter from Section 1.3.3.2. A function f was filtered in Equation (1.10). In a same way it is possible to filter the Taylor expansion of f. The Taylor expansion of f and its filtered version are given by,

$$
\begin{aligned}
f(y) &= f(x) + (y - x)\frac{\partial f(x)}{\partial x} + \frac{1}{2}(y - x)^2\frac{\partial^2 f(x)}{\partial x^2} + \ldots \\
G(f) &= f(x) + \frac{1}{2}\frac{\partial^2 f(x)}{\partial x^2}\int z^2 G(z)\,dz + \ldots + \frac{1}{n!}\frac{\partial^n f(x)}{\partial x^n}\int z^n G(z)\,dz + \ldots \\
&= f(x) + \sum_{l=1}^{\infty}\frac{\alpha_l}{l!}\frac{\partial^l f(x)}{\partial x^l}
\end{aligned}
\tag{2.3}
$$

The filtered version of f follows from conservation property of constance of the filter G. The variable α_l is given by,

$$\alpha_l = \int z^l G(z)\,dz$$

In Equation (2.3) f is the unfiltered function and $G(f)$ the filtered. The residue or terms on the sub-grid could be found from this equation. The Gaussian filter is not local so it is not possible to use a full implementation of the filter in the computation. That is why some terms has to be approximated. This leads to the following equation, derived from Equation (2.3),

$$G(f) = \left(Id + \sum_{l=1}^{\infty} C_l \bar{\Delta}^{2l}\frac{\partial^{2l}}{\partial x^{2l}}\right)f$$

The C_l will be discussed later on. There could be found an kind of approximation for the inverse (as discussed in the previous section) of the right-hand side.

$$f = \left(Id + \sum_{l=1}^{\infty} C_l' \bar{\Delta}^{2l} \frac{\partial^{2l}}{\partial x^{2l}} \right) G(f)$$

which shows that the flow $\mathbf{u}$ could be expressed by using $\bar{\mathbf{u}}$, so it can be used for large eddy simulations. The problem with the Clark model is its instability, especially for small values of ν. We will later look back at the Clark model.

2.2 Scale Residual Method

The scale residual method from professor J. Maurer and professor M. Fey is a two-grid level procedure. It computes the solution of the large eddy simulation and finds each step a suitable model for the sub-grid term. This model is found by minimizing the following residual,

$$E = [\mathcal{NS}, G](\mathbf{u}) - m(G(\mathbf{u})) \tag{2.4}$$

where $m(G(\mathbf{u}))$ is the model for the sub-grid and E is the residual. The residual is minimized by a suitable m, so by finding a suitable model for the sub-grid terms. With this m it is possible to compute a next step in the large eddy simulation. The filter G needs some extra properties to be used for a scale residual method.

- G is a projection. This means that G is idempotent, so $G(x) = G(G(x)) = G(G(G(x))) = \dots$. The spectral cut-off filter is the only filter discussed in Section 1.3.3 which was also a projection.

- G has to commute with the Navier-Stokes equation, which means,

$$\mathcal{NS}(G(\mathbf{u})) = \mathcal{NS}(G(G(\mathbf{u}))) = G(\mathcal{NS}(G(x)))$$

The first equality follows from the first property and the second shows that the G commutes.

With these properties Equation (2.4) can be rewritten as,

$$\begin{aligned} E &= G(\mathcal{NS}(\mathbf{u})) - G(\mathcal{NS}(G(\mathbf{u}))) - m(G(\mathbf{u})) \\ &= G(\mathcal{NS} \circ Id - \mathcal{NS}(G))(\mathbf{u}) - m(G(\mathbf{u})) \end{aligned} \tag{2.5}$$

This follows from the definition of the commutator and because $\mathcal{NS}(G(\mathbf{u})) = \mathcal{NS}(G(G(\mathbf{u}))) = G(\mathcal{NS}(G(\mathbf{u})))$. The next step is to introduce a set of filters G_k with $k \in [0, N]$ and each of these filters has a spectral radius $\bar{\Delta}_k$ such that $0 = \bar{\Delta}_N < \bar{\Delta}_N - 1 \cdots < \bar{\Delta}_0$, so the filter radius increases as k decreases and $\overline{\Delta_N} \equiv Id$. So for $k = N$ it follows that the filter does nothing and for very small k that only the largest eddies remains. We use these filters one by one and after each applied filter follows a residual E_k, which we can derive from Equation (2.5) as,

$$\begin{aligned} E_k &= G_k(\mathcal{NS} \circ G_N - \mathcal{NS}G_k)(\mathbf{u}) - m(G_k(\mathbf{u})) \\ &= G_k \left(\sum_{i=0}^{k-1} (\mathcal{NS}(G_i) - \mathcal{NS}(G_{j+1}))(\mathbf{u}) \right) - m(G_k(\mathbf{u})) \end{aligned} \tag{2.6}$$

To make a model for the sub-grid term m the following two assumptions are needed. First of all we assume that the interaction between to filters is local, which means that the interaction on

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G_i from another filter G_j gets smaller as j gets further from i. The second assumption is that the difference between two following filters gets smaller as we let i increase, so

$$(\mathcal{NS}(G_{i+1}) - \mathcal{NS}(G_i))(\mathbf{u}) = \alpha(\mathcal{NS}(G_i) - \mathcal{NS}(G_{j-1}))(\mathbf{u})$$

With the constant $\alpha < 1$. From these assumptions and Equation (2.6) it follows that,

$$m(G_k(\mathbf{u})) = G_k(\sum_{i=1}^{k} \alpha^j)(\mathcal{NS}(G_k) - \mathcal{NS}(G_{k+1}))(\mathbf{u}) \tag{2.7}$$

With this model for the sub-grid term it is possible to make a better computation for the large eddy simulation. This leads to the following algorithm,

- A short computation is done on two different grids, one on a fine-grid and one on a coarse-grid.

- From the computation on the fine-grid follows from Equation (2.7) a model m for the sub-grid term.

- The model m is added to the source equation.

This algorithm leads to the following iterative equation,

$$\mathbf{u}_k^{n+1} = (\mathcal{NS}_{k,\Delta t}^2 + \omega(\mathcal{NS}_{k,\Delta t}^2 - \mathcal{NS}_{k+1,2\Delta t}^1))\mathbf{u}_k^{n+1}$$

as can be seen in *Large Eddy Simulation for Incompressible Flows* by *P. Sagaut.* [3] With $\mathbf{u}_k^{n+1}$ the $n+1$th solution on the fine-grid with kth level of filtering. The 1 and 2 in $\mathcal{NS}^1$ and $\mathcal{NS}^2$ do not refer to power but to the applications. The parameter ω follows from the α in Equation (2.7).

2.3 Eddy viscosity models

In this section are eddy viscosity models discussed. These models are harder to understand then previous discussed models and that is why we spend more time on these models then on the others. But first we introduce another notation for the Navier-Stokes equation

2.3.1 Closure models

The problem with the filtered Navier-Stokes equation was that it contained terms on the main-grid and the sub-grid. Models which solve these problems are called closure models. A common notation for the Navier-Stokes equation with closure models is the following,

$$\mathbf{v}_t + (\mathbf{v} \cdot \nabla \mathbf{v}) + \nabla \overline{\mathbf{p}} - 2\nu\nabla \cdot S(\mathbf{v}) = -\nabla \cdot \tau(\mathbf{v}) \tag{2.8}$$

The letter $\mathbf{v}$ is used for these models instead of the filtered velocity $\overline{\mathbf{u}}$ to emphasize that these models differ from the original filtered Navier-Stokes equation. Some more changes can be seen when Equation (2.8) is compared to Equation (1.12). The variable S is the symmetric part of the velocity gradient or also called the strain rate tensor. The divergence of this S is similar to the $\Delta\overline{\mathbf{u}}$ term from the filtered Navier-Stokes equation. The whole idea of closure models is to find a suitable choice for τ to model the sub-grid eddies.
An example of a closure model is the Smagorinksy, where τ is given by,

$$\tau(\mathbf{v}) - \frac{1}{3}tr(\tau)I = -2\nu_t S(\mathbf{v}) \quad \text{with} \quad \nu_t = C_S^2 \bar{\Delta}\sqrt{2tr(S^2(\mathbf{v}))} \tag{2.9}$$

The Smagorinksy model is also an eddy viscosity model, which will be explained later on.

Here C_S is a scalar for which different researches had led to different values. The values range from 0.10 to 0.1. [5]. It is also possible to make C_S a dynamical value $C_S(\mathbf{v})$, so ν_t completely depends on $\mathbf{v}$.

The Clark model discussed in Section 2.1.2 is also a closure model and has the following form,

$$\tau(\mathbf{v}) = C_\delta \nabla \mathbf{v}^T \nabla \mathbf{v}$$

2.3.2 Scale separation condition

The elements in the eddy viscosity model may not produce elements on the main-grid which could be influenced by elements on the sub-grid. The following theorems are needed to make sure of this, the Poincaré's inequality and the Gronwall lemma.

- **Poincaré's inequality**
  The Poincaé's inequality states that there exists a C_δ depending only on the region Ω_δ such that,
  $$\|\mathbf{u} - \bar{\mathbf{u}}\| \leq C_\delta \|\nabla \mathbf{u}\|$$
  where $\bar{\mathbf{u}}$ is the average value over Ω_δ, given by
  $$\bar{\mathbf{u}} = \frac{1}{|\Omega|} \int_\Omega \mathbf{u}(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$
  which is also the top hat or boxed filtered version of $\mathbf{u}$. In Ω_δ the δ in the subscript stands for the diameter of the area Ω. It has been shown that the poincaré constant (C_δ) is equal to $(\delta/\pi)^2$, for any convex domain.

- **Gronwall lemma**
  The Gronwall lemma states that if we have for an positive time interval the following bound for the derivative of $\mathbf{u}$,

  $$\frac{\mathrm{d}\mathbf{u}(t)}{\mathrm{d}t} \leq \beta(t)\mathbf{u}(t)$$

  then $\mathbf{u}$ self is bounded by,

  $$\mathbf{u}(t) \leq \mathbf{u}(a)exp\Big(\int_a^t \beta(s) \, \mathrm{d}s\Big)$$

With these two theorems it can be shown that the residual field of $\mathbf{v}$ from Equation (2.8) will be small in a eddy viscosity model. When we looked at filters we had something similar, we had $\mathbf{v} = \bar{\mathbf{v}} + \tilde{\mathbf{v}}$ where $\bar{\mathbf{v}}$ was the term with the eddies bigger then δ and $\tilde{\mathbf{v}}$ the term with eddies smaller then δ. We can look at the Navier-Stokes equation on the sub-scale in a similar way as we did with the filtered Navier-Stokes equation,

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$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathbf{v}} = \nu\Delta\tilde{\mathbf{v}} + t(\bar{\mathbf{v}}, \tilde{\mathbf{v}}) - \nabla\tau'(\mathbf{v})$$

where t is a non linear term which we will not further specify. From this we can derive the energy equation from the sub-scale on Ω_δ. This is done in the same way as in Section 1.5, by first taking an inner product with v' and then take the space average over Ω_δ, where Ω_δ is an area with diameter δ.

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_\delta}\frac{1}{2}\|\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} &= \int_{\Omega_\delta}(\nu(\Delta\tilde{\mathbf{v}}\cdot\tilde{\mathbf{v}}) + T(\bar{\mathbf{v}},\tilde{\mathbf{v}}) - (\nabla\tau'(\mathbf{v})\cdot\tilde{\mathbf{v}}))\,\mathrm{d}\mathbf{x} \\
&= \int_{\Omega_\delta}(\nu\|\nabla\tilde{\mathbf{v}}\| + T(\bar{\mathbf{v}},\tilde{\mathbf{v}}) + (\tau'(\mathbf{v})\cdot\nabla\tilde{\mathbf{v}}))\,\mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.10}
$$

The second term in Equation (2.10) on the right-hand side is the energy transfer from $\bar{\mathbf{v}}$ to $\tilde{\mathbf{v}}$ and the third term is the eddy dissipation. By taking the model for $\nabla\tau$ in such a way that the energy transfer got canceled out, so we get the following equation for the energy transfer,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_\delta}\frac{1}{2}\|\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} = -\nu\int_{\Omega_\delta}\|\nabla\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} \tag{2.11}$$

It can be seen that Equation (2.11) does not depend on $\bar{\mathbf{v}}$ so it is independent of forces from scales greater than δ. By using Poincaré inequality on Equation (2.11) it follows that $-\nu\int_{\Omega_\delta}\|\nabla\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} \leq -\frac{\nu}{C_\delta}\int_{\Omega_\delta}\|\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x}$. Using this with the Gronwall Lemma we get,

$$\int_{\Omega_\delta}\|\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} \leq exp(-2\nu t/C_\delta)\int_{\Omega_\delta}\|\mathbf{v}_0'\|^2\,\mathrm{d}\mathbf{x}$$

where $\mathbf{v}_0' = \tilde{\mathbf{v}}(x,0)$, which is the velocity of the small eddies at the initial time. This follows from the Gronwall lemma with $\beta = -2\nu t/C_\delta$). We can also apply the Poincaré inequality and the Gronwall lemma to $\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_\delta}\frac{1}{2}\|\nabla\mathbf{v}\|^2\,\mathrm{d}\mathbf{x} = -\nu\int_{\Omega_\delta}\|\Delta\mathbf{v}\|^2\,\mathrm{d}\mathbf{x}$. This will result into the following,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_\delta}\frac{1}{2}\|\tilde{\mathbf{v}}\|^2\,\mathrm{d}\mathbf{x} \leq C_\delta\int_{\Omega_\delta}\|\nabla\mathbf{v}\|^2\,\mathrm{d}\mathbf{x} \leq C_\delta exp(-2\nu t/C_\delta)\int_{\Omega_\delta}\frac{1}{2}\|\nabla\mathbf{v}_0\|^2\,\mathrm{d}\mathbf{x} \tag{2.12}$$

So the residual field $\tilde{\mathbf{v}}$ is bounded by the initial gradient of the velocity and will be of insignificant size if we assume that energy from the larger scales and the eddy dissipation cancel each other out. This is equivalent to saying that,

$$
\begin{aligned}
0 &= \int_{\Omega_\delta}(-\nabla((\mathbf{v}\cdot\nabla)\nabla):\nabla\mathbf{v} - \tau:\nabla\Delta\mathbf{v})\,\mathrm{d}\mathbf{x} \\
&\Longleftrightarrow \\
\int_{\Omega_\delta}\tau:S(\Delta\mathbf{v})\,\mathrm{d}\mathbf{x} &= -\int_{\Omega_\delta}\nabla\mathbf{v}^T\nabla\mathbf{v}:S(\mathbf{v})\,\mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.13}
$$

We can not simply take the usual inner product since that is defined for vectors, while the equations here are expressed as matrices. The inner product is then defined by the Frobenius product, which is noted by " : ". The Frobenius norm is an operator from $\mathbb{R}^{3\times 3}$ to $\mathbb{R}$ and is defined by $A:B = tr(AB^T)$. We can write the gradient of the velocity $(\nabla\mathbf{v})$ as the sum of its symmetric part $S(\mathbf{v})$ and its skew-symmetric part $A(\mathbf{v})$ given by $A(\mathbf{v}) = \frac{1}{2}(\nabla\mathbf{v} - \nabla\mathbf{v}^T)$. Equation (2.12) will then become,

$$
\begin{aligned}
\int_{\Omega_\delta}\tau:S(\Delta\mathbf{v})\,\mathrm{d}\mathbf{x} &= -\int_{\Omega_\delta}(S(\mathbf{v}) + A(\mathbf{v}))(S(\mathbf{v}) + A(\mathbf{v}))^T:S(\mathbf{v})\,\mathrm{d}\mathbf{x} \\
&= -\int_{\Omega_\delta}(S(\mathbf{v}) + A(\mathbf{v}))(S(\mathbf{v}) - A(\mathbf{v})):S(\mathbf{v})\,\mathrm{d}\mathbf{x} \\
&= \int_{\Omega_\delta}(A^2(\mathbf{v}) - S^2(\mathbf{v}))^T:S(\mathbf{v})\,\mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.14}
$$

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Equation (2.14) is known as the scale separation condition, since it is the necessary condition to have a balanced dynamic between the smaller and larger eddies.

2.3.3 Scale separation condition and the vorticity equation

We will now try to express the right-hand side of Equation (2.13) in only the strain rate tensor $(S(\mathbf{v}))$. This is done by the enstrophy of the vorticity equation. The vorticity ω of $\mathbf{v}$ is given by $\omega = \nabla \times \mathbf{v}$. To get to the enstrophy of vorticity equation we start with Equation (2.8) and take the curl $(\nabla \times .)$ on both sides.

$$\nabla \times \mathbf{v}_t + \nabla \times (\mathbf{v} \cdot \nabla \mathbf{v}) + \nabla \times \nabla \hat{\mathbf{p}} - \nabla \times 2\nu \nabla \cdot S(\mathbf{v}) = -\nabla \times \nabla \cdot \tau(\mathbf{v})$$

Since the space operator $\nabla \times$ and the time operator $\frac{\mathrm{d}}{\mathrm{d}t}$ do not effect each other we can rewrite the first term to ω_t. We can rewrite the second term as $\nabla \times (\mathbf{v} \cdot \nabla \mathbf{v}) = \omega \cdot \mathbf{v} = \omega \cdot S(\mathbf{v})$. To get the enstrophy equation we take the inner product with ω and take the space average over Ω_δ. It is assumed that p has periodic boundary conditions over Ω_δ so it vanishes. This will result in,

$$
\begin{aligned}
\int_{\Omega_\delta} \omega \cdot \omega_t \, \mathrm{d}\mathbf{x} &= \int_{\Omega_\delta} 2\nu\omega \cdot \nabla \times \nabla S(\mathbf{v}) - \omega \cdot S(\mathbf{v})\omega - \omega \cdot \nabla \times \nabla : \tau(\mathbf{v}) \, \mathrm{d}\mathbf{x} \\
&\Longleftrightarrow \\
\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_\delta} \frac{1}{2}\|\omega\|^2 \, \mathrm{d}\mathbf{x} &= \int_{\Omega_\delta} -\nu\|\nabla\omega\|^2 - \omega \cdot S(\mathbf{v})\omega + \tau(\mathbf{v}) : \nabla(\nabla \times \omega) \, \mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.15}
$$

Getting the derivation out of the integral on the left-hand side follows from a similar process as in Section 1.5. Since it was assumed that there were no boundary terms it can be stated that the curl is self adjoint, so $(\nabla \times \mathbf{v}, \mathbf{u}) = (\mathbf{v}, \nabla \times \mathbf{u})$. From this it follows that,

$$(\omega \cdot \nabla \times \nabla : \tau(\mathbf{v})) = (\nabla \times \omega \cdot \nabla : \tau(\mathbf{v})) = -(\nabla(\nabla \times \omega) : \tau(\mathbf{v}))$$

The equality in Equation (2.15) for the first term in the right-hand side follows from the self-adjointness of the curl operator and noting that the 2 vanishes in the $\frac{1}{2}$ from $S(\mathbf{v})$. Now that we have the vorticity Equation (2.15), we can note some properties which will be needed. In Equation (2.15), $\omega \cdot S(\mathbf{v})\omega$ stands for the vortex stretching which could produce vortices's of scales less than δ and the term with the τ is the eddy dissipation. We want, similar to the energy equation, that these two terms cancel each other out, so we have,

$$\int_{\Omega_\delta} \omega \cdot S(\mathbf{v})\omega \, \mathrm{d}\mathbf{x} = \int_{\Omega_\delta} \tau(\mathbf{v}) : \nabla(\nabla \times \omega) \, \mathrm{d}\mathbf{x}$$

From the identity $\nabla \times \omega = \nabla(\nabla \cdot \mathbf{v}) - \Delta\mathbf{v}$ and $\nabla \cdot \mathbf{v} = 0$ it follows that $\tau(\mathbf{v}) : \nabla(\nabla \times \omega) = -\tau : S(\Delta\mathbf{v})$. With this and Equation (2.14) we see that,

$$\int_{\Omega_\delta} \omega \cdot S(\mathbf{v})\omega \, \mathrm{d}\mathbf{x} = \int_{\Omega_\delta} (A^2(\mathbf{v}) - S^2(\mathbf{v})) : S(\mathbf{v}) \, \mathrm{d}\mathbf{x}$$

By using a consequence of the identity $\omega \otimes \omega = 4A^2(\mathbf{v}) + \|\omega\|^2 I$ as can be read in *On a consistent, scale-truncation model for large eddy simulation* by *R. Verstappen* [4], it follows that $\int_{\Omega_\delta} A^2(\mathbf{v}) : S(\mathbf{v}) \, \mathrm{d}\mathbf{x} = -\frac{1}{3} \int_{\Omega_\delta} S^2(\mathbf{v}) : S(\mathbf{v}) \, \mathrm{d}\mathbf{x}$. This will lead to,

$$
\begin{aligned}
\int_{\Omega_\delta} \tau(\mathbf{v}) : S(\Delta \mathbf{v}) \, \mathrm{d}\mathbf{x} &= \int_{\Omega_\delta} (A^2(\mathbf{v}) - S^2(\mathbf{v})) : S(\mathbf{v}) \, \mathrm{d}\mathbf{x} \\
&= -\frac{4}{3} \int_{\Omega_\delta} tr(S^3(\mathbf{v})) \, \mathrm{d}\mathbf{x} \\
&= 4 \int_{\Omega_\delta} r(\mathbf{v}) \, \mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.16}
$$

Here $r(\mathbf{v})$ is know as the third invariant from the strain rate tensor.

2.3.4 Eddy viscosity models

We will now look once again at the Smagorinsky model (Equation (2.9)). The scale separation condition (Equation (2.14)) expanded with the vorticity equation led to Equation (2.16). For the Smagorinksy model this condition means,

$$
4 \int_{\Omega_\delta} r(\mathbf{v}) \, \mathrm{d}\mathbf{x} = \int_{\Omega_\delta} \tau(\mathbf{v}) : S(\Delta \mathbf{v}) \, \mathrm{d}\mathbf{x} = 2\nu_t \int_{\Omega_\delta} S(\mathbf{v}) : S(-\Delta \mathbf{v}) \, \mathrm{d}\mathbf{x}
\tag{2.17}
$$

The operator $-\Delta$ is symmetric and positive definite on Ω_δ. The smallest eigenvalue of $-\Delta$ is also the inverse of the Poincaré, so $1/C_\delta$. This will lead to,

$$
\int_{\Omega_\delta} S(\mathbf{v}) : S(-\Delta \mathbf{v}) \, \mathrm{d}\mathbf{x} \geq \frac{1}{C_\delta} \int_{\Omega_\delta} S(\mathbf{v}) : S(\mathbf{v}) \, \mathrm{d}\mathbf{x} = \frac{2}{C_\delta} \int_{\Omega_\delta} q(\mathbf{v}) \, \mathrm{d}\mathbf{x}
\tag{2.18}
$$

with q the second invariant of the strain rate tensor. Combining Equations (2.17) and (2.18) will result in the following lowerbound of the eddy viscosity,

$$
\nu_t \geq C_\delta \frac{\overline{r(\mathbf{v})}}{\overline{q(\mathbf{v})}}
\tag{2.19}
$$

where the bar means the space average over Ω_δ. This will give $\tau(\mathbf{v}) \leq -2C_\delta \frac{\overline{r(\mathbf{v})}}{\overline{q(\mathbf{v})}} S(\mathbf{v})$ as model. If we would project this on the tensor $-S(\mathbf{v})$ we will get,

$$
\int_{\Omega_\delta} -2C_\delta \frac{\overline{r(\mathbf{v})}}{\overline{q(\mathbf{v})}} S(\mathbf{v}) : -S(\mathbf{v}) \, \mathrm{d}\mathbf{x} = 2C_\delta \frac{\overline{r(\mathbf{v})}}{\overline{q(\mathbf{v})}} \int_{\Omega_\delta} S(\mathbf{v}) : S(\mathbf{v}) \mathrm{d}x = 4C_\delta \overline{r(\mathbf{v})}
$$

Here we see the Clark model in the right-hand side. So the projection of the Clark model on the tensor $-S(\mathbf{v})$ is equal to the lowerbound of the eddy viscosity models. This can be seen in the next figure.
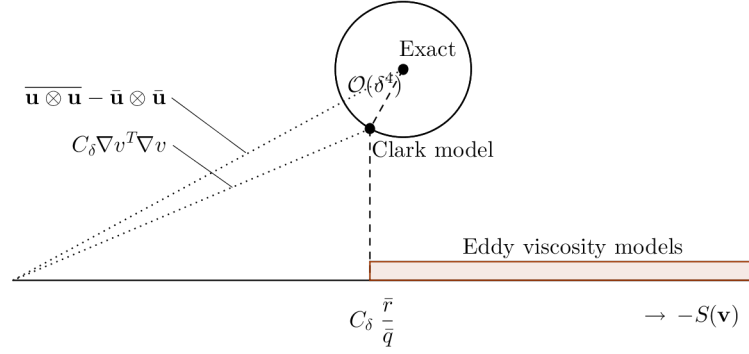
Figure 2.1: The Clark model and the eddy viscosity models

In Figure 2.1 is a schematic representation of the Clark model and the eddy viscosity models. The Clark model is exact up to an order of $\mathcal{O}$, so it lies in the circle with radius $\mathcal{O}$. On the horizontal axis is the tensor $-S(\mathbf{v})$ with all the eddy viscosity models, with in the shaded area all the models which satisfy the scale separation condition. It can be seen that this area starts at the lower bound of these models and that the projection of the Clark model coincides with this bound.

2.3.5 The qr-model

The eddy viscosity models as presented in the previous section still has some issues. The aim of the scale residual method and approximate deconvolution procedure was to get rid of the terms at the sub-grid so they do not have to be computed. The eddy viscosity models are still expressed in $\mathbf{v}$ which still has term which are to expensive to compute. That is why we now will try to write the model in terms of $q(\bar{\mathbf{v}})$ and $r(\mathbf{v})$ instead of $\overline{q(\mathbf{v})}$ and $\overline{r(\mathbf{v})}$. We use the following identities $r \propto Re3/2$ and $q \propto Re^1$. Since $\overline{r(\mathbf{v})}/\overline{q(\mathbf{v})} \propto Re^0$ we get that $\overline{r(\mathbf{v})}/\overline{q(\mathbf{v})}^{3/2} \approx \overline{r(\mathbf{v})}/\overline{q(\mathbf{v})}^{3/2}$. By using this approximation one of the undesired terms can disappear from the lower bound stated in Equation (2.19). Canceling $\overline{r(\mathbf{v})}$ results in,

$$\nu_t \approx C_\delta \frac{|r(\bar{\mathbf{v}})|}{q(\bar{\mathbf{v}})^{3/2}} \overline{q(\mathbf{v})}^{1/2}$$

To get rid of $\overline{q(\mathbf{v})}$ we have to write it out and use Poincaré and the term on the sub-scale $\tilde{\mathbf{v}} = \frac{1}{2}C_\delta \Delta \bar{\mathbf{v}}$.

$$\begin{aligned} \overline{q(\mathbf{v})} &= \tfrac{1}{4}\overline{\|\nabla\mathbf{v}\|^2} = \tfrac{1}{4}\overline{\|\nabla(\bar{\mathbf{v}} - \tfrac{1}{2}C_\delta\Delta\bar{\mathbf{v}})\|^2} \leq \tfrac{1}{4}(1 + \tfrac{1}{2}C_\delta/C_\delta)^2\overline{\|\nabla\bar{\mathbf{v}}\|^2} \\ &= \left(\tfrac{3}{2}\right)^2\overline{q(\bar{\mathbf{v}})} = \left(\tfrac{3}{2}\right)^2 q(\bar{\mathbf{v}}) \end{aligned}$$

Which will give the eddy viscosity model in the lowest order,

$$\nu_t(\mathbf{v}) = \frac{3}{2}\frac{r(\mathbf{v})}{q(\mathbf{v})}$$

This is known as a eddy viscosity qr-model.

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2.4　S squared model

In this section we look at a custom model for this thesis. It is a closure model which has similarities with the previous discussed eddy viscosity model. We saw that the eddy viscosity model was derived from Equation (2.13). From this same equation we derive another model and will see that the new model and the eddy viscosity model form a basis for other models.

2.4.1　The derivation

We recall that Equation (2.13) and $\tau(\mathbf{v}) = -2\nu_t S(\mathbf{v})$ led to the eddy viscosity models. So the eddy viscosity models are all located on the strain rate tensor axis $S(\mathbf{v})$. Another possible choice for τ would be $\tau = \nu_{S^2} S^2(\mathbf{v})$. A suitable ν_{S^2} would result in a projection of the solution on the square of the strain rate. This ν_{S^2} can be found by starting from Equation (2.13) and use the closure model with the square of the strain rate. This results in,

$$
\begin{aligned}
4\int_{\Omega_\delta} r(\mathbf{v})\, \mathrm{d}\mathbf{x} &= \int_{\Omega_\delta} \tau : S(\Delta \mathbf{v})\, \mathrm{d}\mathbf{x} \\
&= \int_{\Omega_\delta} \nu_{S^2} S^2(\mathbf{v}) : S(\Delta \mathbf{v})\, \mathrm{d}\mathbf{x}
\end{aligned}
\tag{2.20}
$$

Similar to how Equation (2.17) led to the eddy viscosity models, it can be seen that Equation (2.20) leads to the following definition for ν_{S^2},

$$
\nu_{S^2} = \frac{4\int_{\Omega_\delta} r(\mathbf{v})\, \mathrm{d}\mathbf{x}}{\int_{\Omega_\delta} S^2(\mathbf{v}) : S(\Delta \mathbf{v})\, \mathrm{d}\mathbf{x}}
\tag{2.21}
$$

So $\tau = \nu_{S^2} S^2(\mathbf{v})$ and Equation (2.21) form another large eddy simulation closure model. An example of a squared strain rate tensor model will be tested in the research section of this thesis.

2.4.2　Basis for higher order models

A natural question which arises from the the eddy viscosity model and the S squared model is if it is possible to make a model based of $S^3(\mathbf{v})$ or of an even higher order. The answer to this question follows from the invariants of the strain rate tensor. The three invariants for the three times three symmetric matrix A are,

$$
I_A = tr(A) \qquad II_A = \frac{1}{2}(((tr(A))^2 - tr(A^2))) \qquad III_A = det(A)
$$

And from the Cayley-Hamilton theorem it follows that,

$$
A^3 - I_A A^2 + II_A A - III_A I = 0
\tag{2.22}
$$

with I the identity matrix. Since the strain rate matrix S is also a symmetric matrix it follows that the previous equations also hold for S. The first invariant of S (I_S) is the trace, which is the same as $2\nabla \cdot \mathbf{v}$, which we recall from Equation (1.2) to be zero. From the first invariant it follows that the second invariant (II_S) is simplified to $\frac{-1}{2} tr(S^2)$, which was discussed in Equation (2.18) and was called $q(\mathbf{v})$. And the third strain rate tensor was already defined in Equation (2.16). So Equation (2.22) for S becomes,

$$
S^3 - qS + rI = 0
$$

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From this equation it follows that every closure model with a power of the strain rate tensor higher then three, can be written as the sum of a terms of the strain rate tensor, it first square and I. As an example it can be seen that $S^5 = S^2(S^3) = S^2(qS - rI) = qS^3 - rS^2 = q(qS - rI) - rS^2 = q^2S - rS^2 - qrI$. This is just an example and any other closure model with a power of S can be expressed in I,S and S^2.

3: Research on different large eddy simulation models

In this research we will look at some large eddy simulations of a turbulent flow through a channel. The following figure shows the mean velocity profile of a simulation through a channel,
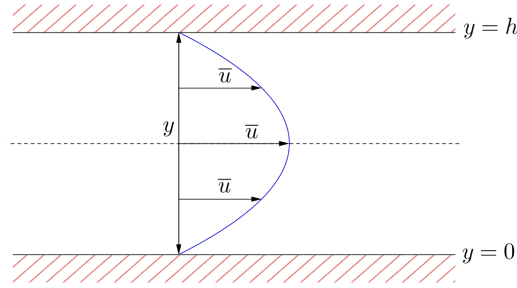
Figure 3.1: A velocity profile in a channel flow

We try to model this problem with three different large eddy simulation models and compare their results. Two of the three models which will be used were discussed in Chapter 2.

Clark model: The approximate deconvolution method which was discussed in Section 2.1.2.

Qr-model: The eddy viscosity model which was discussed in Section 2.3.5.

Squared S model model: We have seen that Eddy viscosity models were described on the strain rate tensor. This model is a projection just like the eddy viscosity model, but its projection is not on the $S(\mathbf{v})$ axis, but on the $S^2(\mathbf{v})$ axis.

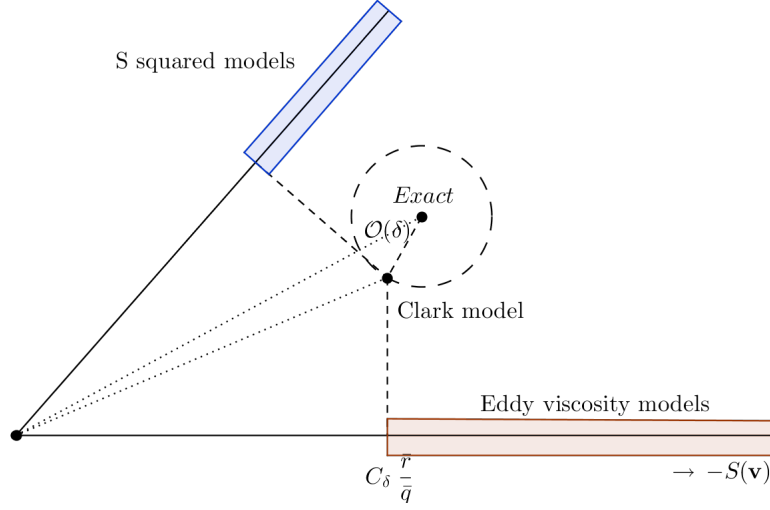In the next figure we see a schematic representation of all three models.

Figure 3.2: A representation of the Clark model, the qr-model and the S squared model

The data from these models is compared to a direct numerical solution (DNS) of the Navier-Stokes equation of this problem. The DNS data is from the computation by R.D. Moser, J. Kim and N.N. Mansour.

3.1   Law of the wall

The DNS data from R.D. Moser, J. Kim and N.N. Mansour gives a numerical approach for the mean velocity at some point in the fluid. To test if this data makes any sense we need some more theory. This way we not only know if the LES data fits the DNS data, but also if it is maybe even better at some points. That is why we need two more theorems to compare the DNS and the LES data with. The first theorem states that the flow is laminar near the boundaries, which means that there will not be any turbulence in this region and $\mathbf{u}$ is only determined by y. The relation is the following.

$$\mathbf{u}^+ = y^+ \quad \text{with} \quad y^+ = \frac{y\mathbf{u}_\tau}{\nu} \quad \mathbf{u}^+ = \frac{\mathbf{u}}{\mathbf{u}_\tau}$$

It can be seen that the variables are scaled to make them dimensionless, but not in the same way as in Section 1.1.3. The only new variable is $\mathbf{u}_\tau$, which is the friction velocity. The region near the wall where the flow is near laminar is called the viscous sublayer. The second theorem is the Law of the wall, stated in 1930 by Th. van Kármán. [7]. The law states that in a turbulent flow the average velocity is proportional to the logarithm of the distance to the boundary. Since it involves the logarithm of the distance to the wall, this theorem is also called the Log Law. This theorem only applies for a small partition of the flow, which is called the log-law region. In this region we can define $\mathbf{u}^+$ with,

$$\mathbf{u}^+ = \frac{1}{0.41} \ln y^+ + C^+$$

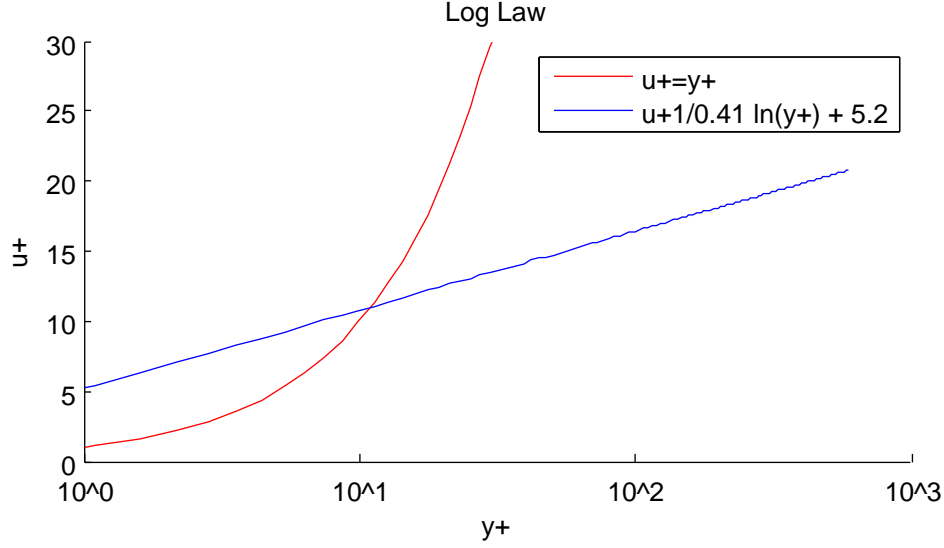These two theorems lead to the following figure,

Figure 3.3: The law of the wall

We suspect that in the data will fit to the red line in the first part of the plot, which is the viscous sublayer, and will match the blue line in the log-law region.

3.2 The Program

In this section there will be a description of some aspects of the program used for this research. The code is written in Fortran, which is imperative programming language used for numerical computations. It is commonly used in computational fluid dynamics and other areas like numerical weather prediction. The main program is called *LES* and it calculates the flow on a three dimensional grid. The program originally only used the qr-model, but with some adjustments it was possible to also use the Clark model instead. The S squared model required some more adjusments, but was also possible to program.

3.2.1   Parameters

Our computations are done on a grid with 64 grid points in each direction on a three dimensional domain. Other parameters which can be altered in *LES* are the direction and the mass of the flow, the order of the spatial discretization, the amount and length of the time steps and the tolerance of the Poisson solver. In this research we will only adjust the amount of time steps and we have set the Reynolds number to 590. In this way the circumstances are similar as those of the program used for DNS data.

3.2.2 Discretization

In this section the discretization for the strain rate matrix is explained. Other elements are discretized in the same way. The matrix of the strain rate tensor is given by the symmetric part of the gradient of the velocity. So for the three dimensional velocity vector the three times three dimensional strain rate matrix becomes,

$$S(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T) = \frac{1}{2} \begin{pmatrix} 2\frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} & \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \\ \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} & 2\frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \\ \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} & \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} & 2\frac{\partial w}{\partial z} \end{pmatrix}$$

Since the program can not compute the gradient exactly it is necessary to make the following approximation,

$$\frac{\partial u(x - \frac{1}{2}\Delta x, y, z)}{\partial x} \approx \frac{u(x, y, z) - u(x - \Delta x, y, z)}{\Delta x} \tag{3.1}$$

which is called a central approximation of the derivative in $u(x, y, z)$. This can be implemented in a program by making a grid. Figure 3.4 explains how to compute the derivatives in matrix S but only in the two dimensional case, but the approach for the three dimensional model is similar. The grid exists from horizontal en vertical lines given by $x = x_i$ and respectively $y = y_j$. This model permits an non uniform grid, so the distance between each x_i's and between each y_j's does not have to be equal.
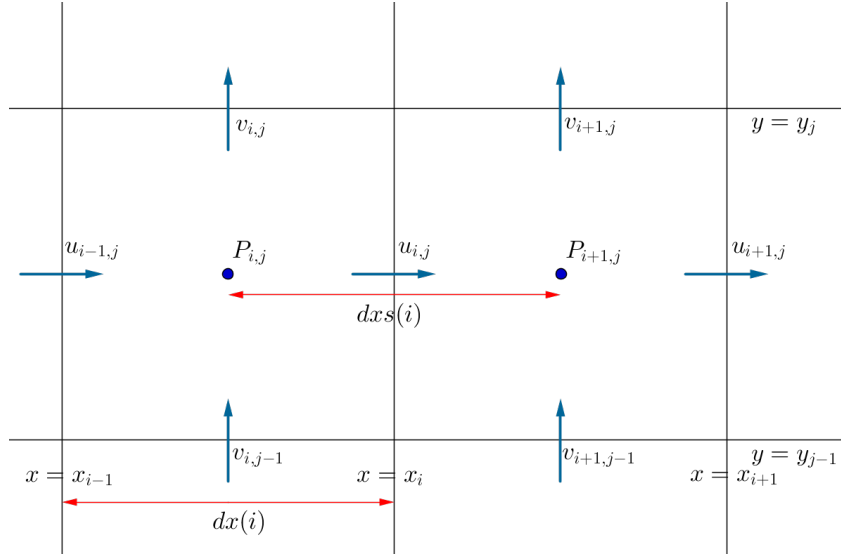

Figure 3.4: The grid

Here the cell-centered points P are the points of the strain rate tensor which are computed. The velocity u is in the direction of the x-axis and y in the direction of the y-axis. the $dx(i)$ stands for the distance between the lines x_i and x_{i-1} and $dxs(i)$ for the distance between the points $P_{i,j}$ and $P_{i+1,j}$. The derivatives $\frac{\partial u}{\partial x}$, $\frac{\partial v}{\partial y}$ and in case of our three dimensional model also, $\frac{\partial w}{\partial z}$ can all be done

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with the earlier discussed backward approximation given in Equation (3.1), since these derivations are in the directions of their velocity's. These derivatives are the components $S(1,1)$, $S(2,2)$ and $S(3,3)$ in the strain rate matrix. For the other components we need a different approach. We will work out one term and the rest can be seen in a similar way. We look at $S(1,2)$ at the point $P_{i,j}$. Here we see the derivative $\frac{\partial v}{\partial x}$ which is expressed in the velocity v and the derivative is taken in the direction of x, so they are in different directions. To get this right we first take the average of $v_{i+1,j}$ and $v_{i+1,j-1}$, which should lay in point $P_{i+1,j}$ and the average of $v_{i-1,j}$ and $v_{i-1,j-1}$, which should lay in point $P_{i-1,j}$ (these last three points can not be seen in Figure 3.4). The points $P_{i-1,j}$, $P_{i,j}$ and $P_{i+1,j}$ are all on the line y_j, so the derivative in $P_{i,j}$ is given by,

$$
\frac{\partial v}{\partial x} \quad \approx \quad \frac{\frac{v_{i+1,j}+v_{i+1,j-1}}{2} - \frac{v_{i-1,j}+v_{i-1,j-1}}{2}}{dxs(i) + dxs(i-1)}
$$

$$
= \quad \frac{v_{i+1,j} + v_{i+1,j-1} - v_{i-1,j} - v_{i-1,j-1}}{2(dxs(i) + dxs(i-1))}
$$

To complete the rest of $S(1,2)$ it is also needed to compute $\frac{\partial u}{\partial y}$, which can be derived in a similar way. Note also that the strain rate tensor is symmetric, so $S(1,2) = S(2,1)$. The elements $S(1,1)$ and $S(1,2)$ have the following form in Fortran,

```
      s(1,1) = (u(i,j,k) - u(i-1,j,k))/dx(i)

      s(1,2) = (v(i+1,j,k) + v(i+1,j-1,k) - v(i-1,j,k)
     &          - v(i-1,j-1,k)) / (4.0D0*(dxs(i)+dxs(i-1)))
     &        + (u(i,j+1,k) + u(i-1,j+1,k) - u(i,j-1,k)
     &          - u(i-1,j-1,k)) / (4.0D0*(dys(j)+dys(j-1)))
```

4: The results

In this section the following results are presented and discussed,

- The DNS data. These results were not computed for this thesis, but will still be discussed.

- The eddy viscosity model.

- The Clark model

- The S squared model.

Of all the models it will discussed how they fit the theoretical frame from the law of the wall and how well they do in comparison to the others.

4.1 Direct Numerical Solution

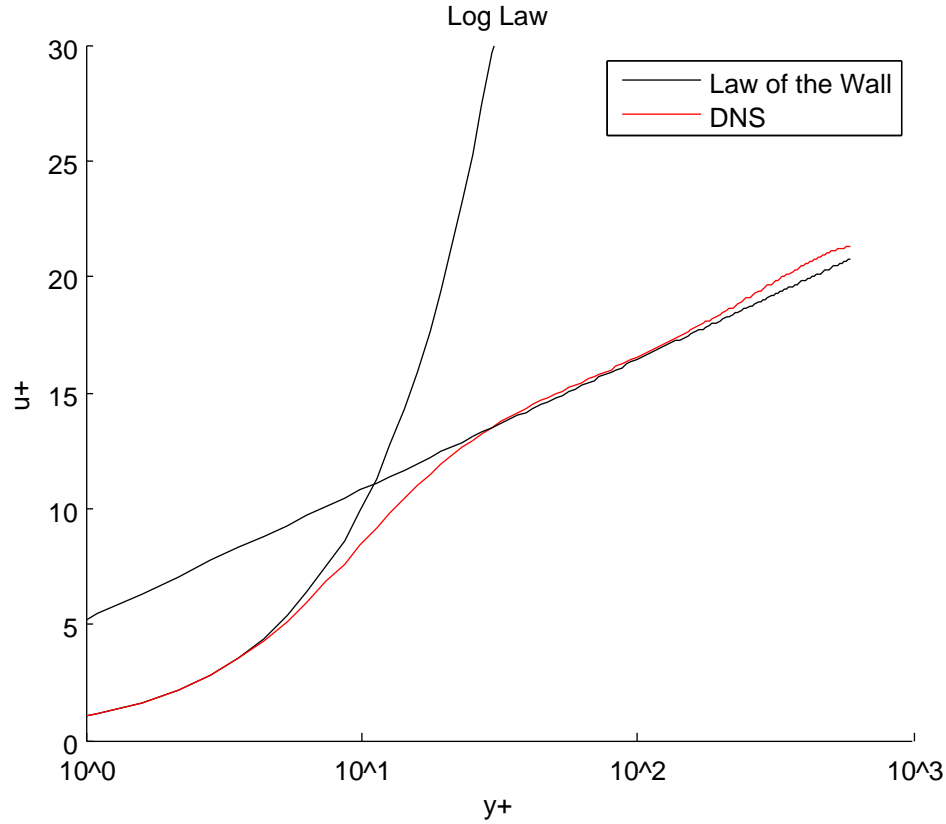We look at the law of the wall and the dataset from the DNS.

Figure 4.1: The direct numerical simulation

We see that the data DNS data fits the theory well in the domain between 10^0 and $10^{\frac{1}{2}}$, which we recall as the viscous sublayer which was discussed in Section 3.1. Later on in the domain between $10^{\frac{1}{2}}$ and 10^3 we see that the data fits the log law curve. This is in the log-law region and it can indeed be seen that the data meets the theory of the log-law. The domain between the viscous sublayer and the log-law region is the buffer layer.
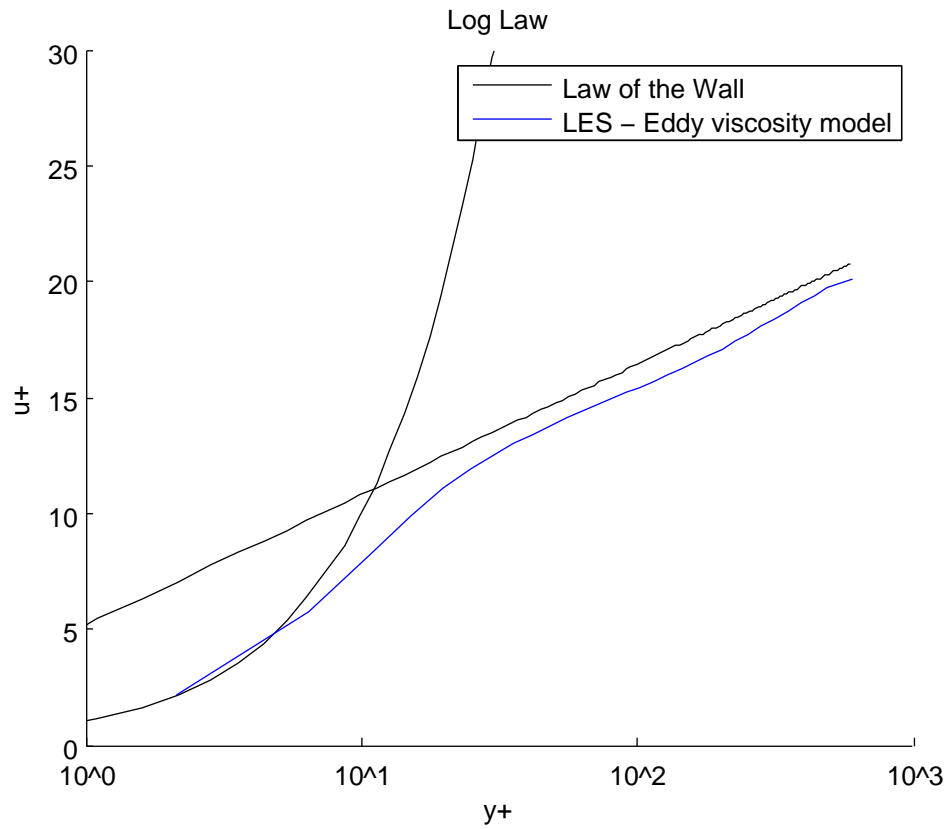
4.2 Eddy Viscosity Model

Figure 4.2: The eddy viscosity model

It can be seen that eddy viscosity model has the good shape, but still has some problems in the low-law region. The DNS data is very close on the theory in the log-law region, where the eddy viscosity model still lays some distance below it.
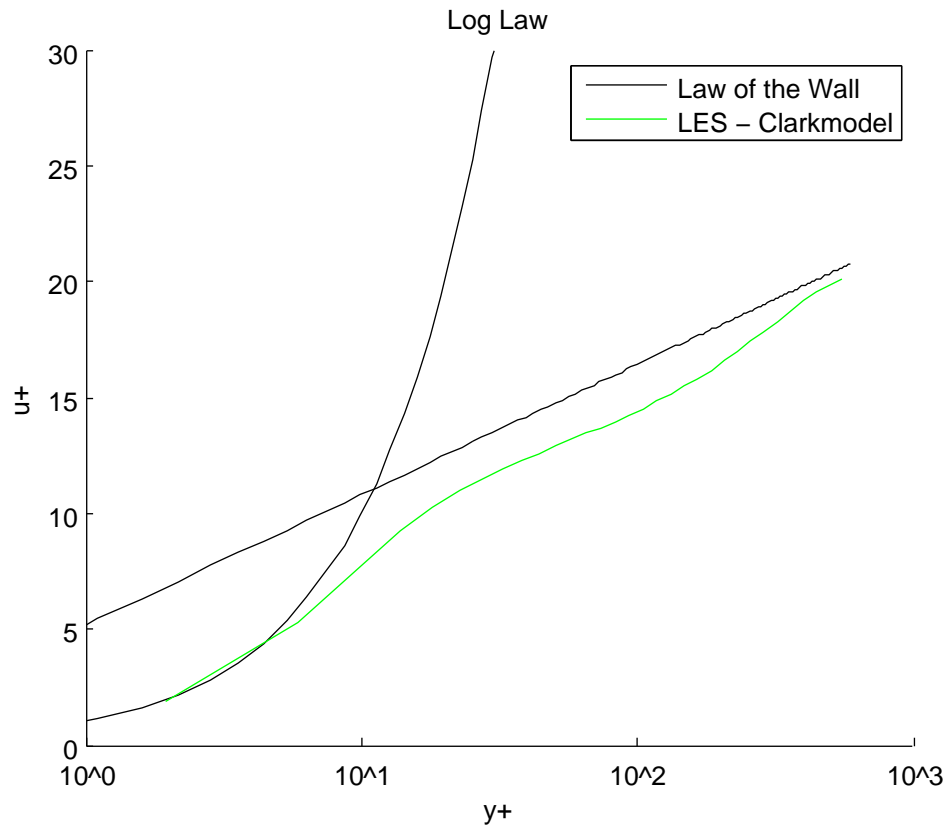
4.3   Clark Model

Figure 4.3: The Clark model

It can be seen that the Clark model fits the theorem in the viscous sublayer, but fails in the log-law region. So the Clark model gives a proper representation of the flow near the wall, maybe even better than the eddy viscosity model, but fails in the region from the wall in comparison with the eddy viscosity model.
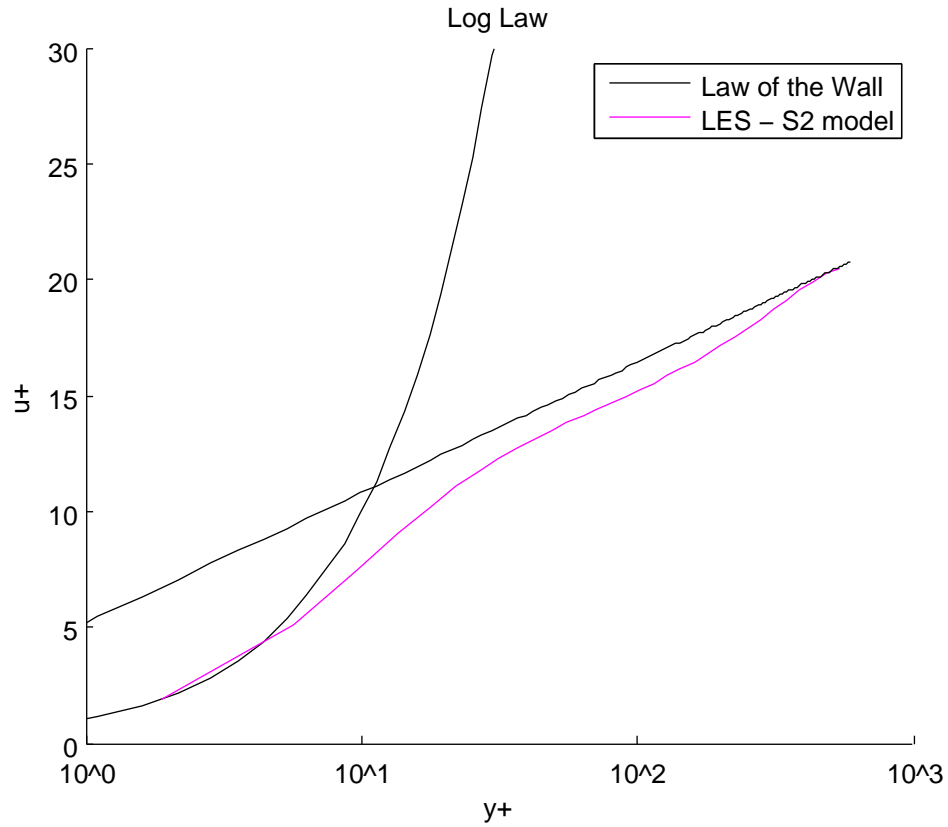
4.4 S squared model

Figure 4.4: The S squared model

Theoretical we saw that S squared model is very similar to the eddy viscosity models and it turns out that their results are very similar. The data of the squared S model fits the theoretical frame of the wall of the law very good in the distance near the wall and just like the eddy viscosity model not perfect in the log-law region. The S squared model seems to fit slightly less than the eddy viscosity model in the beginning of the log-law region, but surpasses it near the end, where it even seems better than the DNS data.

5: Conclusion

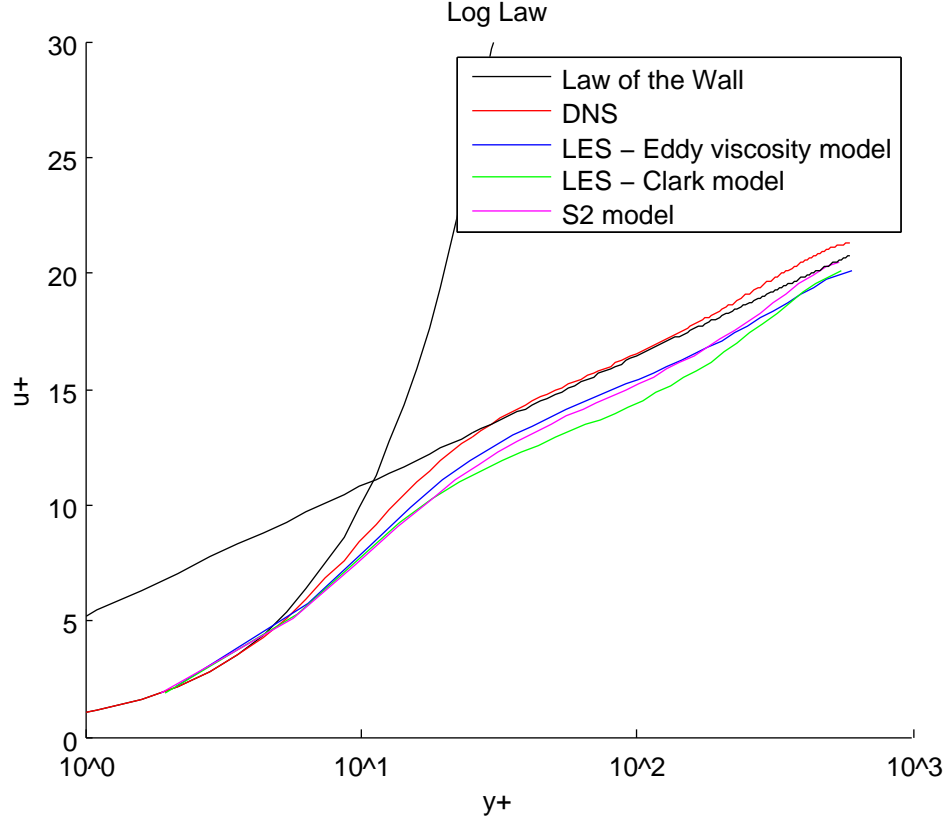In Figure 5.1 we see all the tested models versus the law of the wall and the DNS data.

Figure 5.1: All the tested models compared to the wall-law and DNS data

We see that from all the computations it turns out that the Clark model was the least proper model for this computation. It did however still had the right shape so the model was not wrong. Since the Clark model is an ADP it follows that the model could be improved by producing a better approximated inverse for the convolution filter. However, this also means that the method will take longer to compute and if the method becomes too intense it should be better to go with a direct numerical approach.

The eddy viscosity model and the S squared model were both better than the Clark model and both made a decent computation of the wall of the law. It could be that a combination of these two models will result in an even better model, since it was discussed in Section 2.4 that these two model give a opportunity for other closure models expressed in the strain rate tensor S. Finding an optimal model from the eddy viscosity model and the S squared model is a further subject of research, as is finding the optimal closure model.

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Appendix A: Derivation of the scale-by-scale budget equation

We start with the Navier Stokes equation in the frequency domain and take the inner product defined by

$$(\mathbf{f}, \mathbf{u}_{\kappa_1,\kappa_2}) = \int_V \mathbf{f} \cdot \mathbf{u}_{\kappa_1,\kappa_2} \, \mathrm{d}\mathbf{x}$$

Taking this inner product with the Navier Stokes equation in the frequency domain as in Section 1.2.1 results in.

$$(\frac{\mathrm{d}\mathbf{u}_{\kappa_1,\kappa_2}}{\mathrm{d}t}, \mathbf{u}_{\kappa_1,\kappa_2}) + (P(\mathbf{u} \cdot \nabla \mathbf{u}), \mathbf{u}_{\kappa_1,\kappa_2}) - \nu(\Delta \mathbf{u}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) = (\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) \qquad \text{(A.1)}$$

We want to show that Equation (A.1) equals the scale-by-scale budget equation, given by

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 + \nu|\nabla \mathbf{u}_{\kappa_1,\kappa_2}|^2 = (\mathbf{f}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) + \mathbf{e}_{\kappa_1}(\mathbf{u}) - \mathbf{e}_{\kappa_2}(\mathbf{u})$$

We see that the term with the force $\mathbf{f}_{\kappa_1,\kappa_2}$ did not change much. Since this term represents the force injected by external forces we call this term the total energy injection, similar as in *Turbulence* from *U. Frisch*. [6]. We will now derive the other components term by term.

A.1 Total energy

We start with the first term and we have to prove that

$$(\frac{\mathrm{d}\mathbf{u}_{\kappa_1,\kappa_2}}{\mathrm{d}t} \cdot \mathbf{u}_{\kappa_1,\kappa_2}) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}_{\kappa_1,\kappa_2}|^2$$

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}_{\kappa_1,\kappa_2}|^2 &= \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{u}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) \\
&= (\frac{\mathrm{d}\mathbf{u}_{\kappa_1,\kappa_2}}{\mathrm{d}t}, \mathbf{u}_{\kappa_1,\kappa_2}) + (\mathbf{u}_{\kappa_1,\kappa_2}, \frac{\mathrm{d}\mathbf{u}_{\kappa_1,\kappa_2}}{\mathrm{d}t}) \\
&= 2(\frac{\mathrm{d}\mathbf{u}_{\kappa_1,\kappa_2}}{\mathrm{d}t}, \mathbf{u}_{\kappa_1,\kappa_2})
\end{aligned}$$

Dividing both sides by 2 indeed gives us Equation (A.1). This term is called the total energy. [6]

A.2 Total enstrophy

Next, we proof that,

$$-\nu(\Delta\mathbf{u}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) = \nu|\nabla\mathbf{u}_{\kappa_1,\kappa_2}|^2$$

This follows from a property of the Laplacian. The adjoint of the gradient is $(\nabla f, g) = -(f, \nabla g)$. Since the Laplacian is given by $\Delta f = \nabla^2 f$, it follows that $(\Delta f, g) = (\nabla^2 f, g) = -(\nabla f, \nabla g)$. So it follows that,

$$\begin{aligned}
-(\Delta\mathbf{u}_{\kappa_1,\kappa_2}, \mathbf{u}_{\kappa_1,\kappa_2}) &= -\int_V \Delta\mathbf{u}_{\kappa_1,\kappa_2} \cdot \mathbf{u}_{\kappa_1,\kappa_2} \, \mathrm{d}\mathbf{x} \\
&= \int_V \nabla\mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla\mathbf{u}_{\kappa_1,\kappa_2} \, \mathrm{d}\mathbf{x} \\
&= (\nabla\mathbf{u}_{\kappa_1,\kappa_2}, \nabla\mathbf{u}_{\kappa_1,\kappa_2}) \\
&= |\nabla\mathbf{u}_{\kappa_1,\kappa_2}|^2
\end{aligned}$$

This term is called the total enstrophy. [6]

A.3 Energy flux

All what is left to to is to define $\mathbf{e}_{\kappa_1}(\mathbf{u}) - \mathbf{e}_{\kappa_2}(\mathbf{u})$. We first note that $\mathbf{u} = \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_2,\infty}$, since every piecewise bounded function can be expressed in frequencies, or in our case in wave numbers.

$$(P(\mathbf{u}\cdot\nabla\mathbf{u}), \mathbf{u}_{\kappa_1,\kappa_2}) = ((\mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_2,\infty})\cdot\nabla(\mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_2,\infty}), \mathbf{u}_{\kappa_1,\kappa_2}) \qquad \text{(A.2)}$$

By using $(\nabla f, g) = -(f, \nabla g)$ a multiple times this can be simplified in the following way,

$$
\begin{aligned}
(\mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_2,\infty}) \cdot \nabla \mathbf{u} &= \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u} + \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u} \\
&= \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} \\
&+ \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{0,\kappa_1} \\
&+ \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} \\
&+ \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} \\
&+ \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} \\
&= \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} \\
&+ \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} - \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} \\
&+ \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} \\
&- \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} - \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} \\
&+ \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} \\
&= \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} \\
&+ \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty}
\end{aligned}
$$

From $(\nabla f, g) = -(f, \nabla g)$ it also follows that $(\nabla f, f) = -(f, \nabla f) = 0$. So we have,

$$
\mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_1,\kappa_2} \cdot \nabla \mathbf{u}_{\kappa_1,\kappa_2} + \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty} = \mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty}
$$

So Equation (A.2) results in,

$$
\begin{aligned}
(P(\mathbf{u} \cdot \nabla \mathbf{u}), \mathbf{u}_{\kappa_1,\kappa_2}) &= (\mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1} + \mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty}, \mathbf{u}_{\kappa_1,\kappa_2}) \\
&= (\mathbf{u}_{0,\kappa_1} \cdot \nabla \mathbf{u}_{0,\kappa_1,\infty}, \mathbf{u}_{\kappa_1,\kappa_2}) + (\mathbf{u}_{\kappa_2,\infty} \cdot \nabla \mathbf{u}_{\kappa_2,\infty}, \mathbf{u}_{\kappa_1,\kappa_2}) \\
&= \mathbf{e}_{\kappa_1}(\mathbf{u}) - \mathbf{e}_{\kappa_2}(\mathbf{u})
\end{aligned} \tag{A.3}
$$

Where $\mathbf{e}_{\kappa_1}(\mathbf{u})$ equals the first inner product of Equation (A.3) and $\mathbf{e}_{\kappa_2}(\mathbf{u})$ the second. What is interesting about these two terms is that they do not depend on the internal wavelengths, but only on the boundaries. They represent the energy transport between the wave numbers κ_1 and κ_2.