Modelling Turbulent Flow Using Large Eddy Simulation

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Contents

Chapter 1

Introduction

Turbulent flow is an integral part of the world around us. One can easily observe its effects, from irregular motions arising in fast flowing streams to unexpected gusts of wind inverting poorly made umbrellas. When trying to understand the behaviour of air, whether that be in predicting the weather or in applications of aeronautical engineering, modelling turbulence is particularly important. Despite this, turbulent flow is one of the most poorly understood topics in mathematical physics, and this makes simulating it very difficult.

The difficulties inherent in understanding turbulent flow stem from the equations used to study the motion of fluids. In this dissertation, we will consider an incompressible viscous fluid with unit density and use the Navier–Stokes equations (NSEs) in the following conservation form:

$$\nabla \cdot \mathbf{u} = 0, \tag{1.1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F}. \tag{1.2}$$

As usual, $\mathbf{u} = (u_1, u_2, u_3)^T$ is the flow velocity, p is the pressure, ν is the kinematic viscosity of the fluid, and $\mathbf{F}$ is any body force acting on the fluid. The second term of the momentum equation (1.2) is the divergence of the second-rank tensor $u_i u_j$. Due to the nonlinearity introduced by this term, finding even slightly general solutions to the NSEs is incredibly difficult. Knowledge of qualitative properties of solutions to the full Navier–Stokes equations in 3-D is also extremely limited. Proving "Existence and Smoothness of the Navier–Stokes Equation" is one of the six unsolved 'Millenium Prize Problems' established by the Clay Mathematics Institute (Fefferman, 2000; Ladyzhenskaya, 2003). Progress in this area has mostly been limited to work on related systems with better regularity, an idea pioneered by Leray (1934).

In high Reynolds number flows, turbulence often arises. Although there is no standard definition of turbulence, it is often defined by its flow properties. For example, Sagaut *et al.* (2013) list the most widely agreed of these features as:

- Unpredictability: due to the irregular nature of the solution for a turbulent flow, which exhibits strong dependence on initial and boundary conditions, obtaining a deterministic description of the motion of a turbulent flow is almost impossible;
- Three-dimensionality of the vorticity fluctuations;
- Enhanced mixing: turbulence causes far more rapid mixing than that caused by molecular diffusion, leading to faster mass, momentum and energy transfer;

- Turbulent eddies (or fluctuations) occur over a wide range of scales in both time and space.

Given the analytical intractability of the Navier–Stokes equations outside very special cases, Computational Fluid Dynamics (CFD) has become an increasingly important tool for predicting flows in both scientific and engineering applications. Because of the unpredictable nature of turbulent flow, performing a numerical simulation seems to be the only approach for investigating high Reynolds number flows which may exhibit turbulence. However, the final property mentioned above means that modelling turbulent flow is a multiscale problem with a large separation between the smallest and largest scales of flow features. To reliably perform a Direct Numerical Simulation (DNS) of the NSEs we would need our mesh spacing to be at least as small as the minimum scale at which we expect to observe turbulent eddies.

To investigate how small this minimum scale must be, we introduce the idea of an energy cascade, which was first proposed by Richardson (1922). Let E_K be the kinetic energy of the system, as averaged over a statistically steady state so we have no time dependence. Plancherel's identity tells us that

$$E_K \equiv \frac{1}{2}\int_{\mathbb{R}^3} |\mathbf{u}(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} = \frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3} |\hat{\mathbf{u}}(\mathbf{k})|^2 \,\mathrm{d}\mathbf{k}, \tag{1.3}$$

where $\hat{\mathbf{u}}$ is the Fourier transform of the flow velocity $\mathbf{u}$, as defined in (2.11) below. We can rewrite this last expression as an integral over the scalar wavenumbers $k = |\mathbf{k}|$:

$$E_K = \frac{1}{(2\pi)^3}\int_0^\infty E(k)\,\mathrm{d}k, \quad \text{where} \quad E(k) = \frac{1}{2}\int_{|\mathbf{k}|=k} |\hat{\mathbf{u}}(\mathbf{k})|^2 \,\mathrm{d}S_k, \tag{1.4}$$

and the second integral is over the spherical surface $|\mathbf{k}| = k$. This defines the energy spectrum $E(k)$, which represents the kinetic energy contained in the eddies whose size corresponds to the wavenumber k in spectral space. A typical log-log plot of $E(k)$ against k obtained from experimental results is shown Figure 1.1.

Three distinct regions are visible on this graph, as in Sagaut *et al.* (2013):

- The large scale region (i.e. small k) where the gradient is positive. Here turbulent energy is supplied by large-scale forcing to maintain the statistically steady state.

- The central region where energy is transferred, on average, from larger scales to smaller scales by nonlinear interactions.

- The small scale region where the effective Reynolds number is now small, so viscous effects dissipate the kinetic energy.

The development of a mathematical theory to try to explain turbulence stems mainly from early work on the subject by Kolmogorov (1941). Although progress has been made using this work as inspiration, it is mostly based on experimental evidence such as the energy cascade. Berselli *et al.* (2006) even refer to Kolmogorov's theory as combining "audacious physical guesswork and dimensional analysis." Kolmogorov (1962) later refined his theory by introducing the idea of "intermittent" turbulence, but that is outside the scope of this dissertation. Nonetheless, the phenomena which Kolmogorov (1941) tried to explain are of great significance to the understanding of turbulent flows.

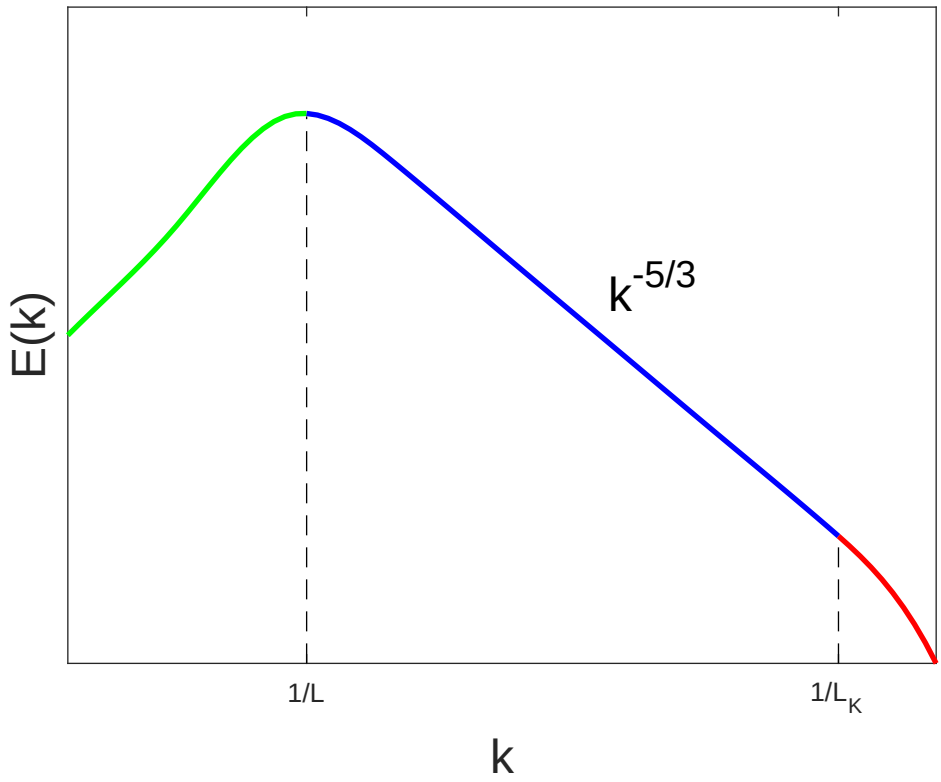

Figure 1.1: Typical log-log plot of the energy spectrum showing the three distinct regions as different colours. The inertial range is displayed in blue, while the large and small scale regions are coloured green and red respectively.

The central region in Figure 1.1, often referred to as the inertial range, is of the most interest. The width of this inertial range increases with $Re = LU/\nu$, the macroscopic Reynolds number of the flow where L and U are appropriate length and velocity scales. Kolmogorov (1941) used dimensional analysis to show that the smallest length scale at which turbulent eddies persist, i.e. where viscous dissipation first becomes important, is $L_K \approx Re^{-3/4}L$. This corresponds to where the small scale region in red appears on the above plot. This is an important result since it tells us the size of the mesh required to accurately simulate the full motions of the flow. For a 3-D DNS, the number of grid points must therefore be $O(Re^{9/4})$. For many applications this makes performing a DNS infeasible. Using typical values of Re for air flow around a car means $\sim 10^{13}$ mesh points are required, and this figure rises to $\sim 10^{45}$ for atmospheric flows (Berselli *et al.*, 2006).

The plot in Figure 1.1 shows a universal relation $E(k) \propto k^{-5/3}$ in the inertial range. Since this relation is observed in most examples of turbulent flow, any model we use to simulate turbulence will want to exhibit this behaviour. Let us define the average kinetic energy flux to smaller scales as

$$\epsilon = 2\zeta k^2 E(k), \tag{1.5}$$

where ζ is the 'eddy turn-over frequency' at wavenumber k, which only depends on k and U by the dimensional relation

$$\zeta \sim kU. \tag{1.6}$$

Manipulating the Fourier transform of the NSEs produces an equation for the energy spectrum of the form

$$\frac{\partial E(k)}{\partial t} = P(k) - \frac{\partial \epsilon}{\partial k} + D(k), \tag{1.7}$$

where $P(k)$ accounts for the large scale energy supply, and $D(k) = -2\nu k^2 E(k)$ accounts for viscous dissipation at small scales. Kolmogorov (1941) hypothesised that in isotropic turbulence (turbulence that looks the same under spatial translations and rotations), both of these terms are negligible in the inertial range, so averaging over statistically steady states tells us that

$$\frac{\partial \epsilon}{\partial k} = 0. \tag{1.8}$$

Thus, if we assume $E(k)$ only depends on k and U, then definitions (1.4) and (1.5) give the dimensional results $E(k) \sim kU^2$ and $\epsilon \sim \zeta k^2 E(k)$, although ϵ is in fact independent of k. Together with the relation (1.6), these imply

$$E(k) = K_0 \epsilon^{2/3} k^{-5/3}, \tag{1.9}$$

where K_0 is a dimensionless constant which has been found to take a value of approximately 1.5 (Sagaut, 2006).

Most applications of CFD are interested in macroscopic quantities, such as the total drag exerted by the flow on an object. It would thus make sense to calculate average flow quantities on a coarser grid to reduce computational cost while hoping to retain the accuracy of the simulation. Reynolds (1895) introduced the concept of evaluating average flow quantities directly over a century ago, and much progress has been made since. This dissertation will focus on Large Eddy Simulation (LES), which involves taking spatial averages of the flow quantities to simulate the large scale motion of the flow. LES has been used since the 1960s, with Smagorinsky (1963) being one of its first uses. However, since LES research has mainly been focused on applications, advances have often been made before the underlying mathematics has been fully understood, particularly regarding the properties of averages.

This dissertation will develop the ideas of filtering and subgrid-scale modelling used in the LES approach. I will describe the conditions that a plausible subgrid model should satisfy, including Galilean invariance and the realizability of the subgrid-scale stress tensor. I will also investigate the possible application of material frame-indifference to LES models. Making assumptions based on these conditions, I will derive the simple Smagorinsky eddy viscosity model, which aims to replicate the effect of the energy flux ϵ at the grid scale using a diffusive term. I will also derive newer dynamic models based on the Germano identity, which motivates the introduction of a further 'test filter' to determine the eddy viscosity during the simulation. Finally, I will describe the relation between the LES approach and the regularization procedure of Leray (1934) for proving the existence of weak solutions of the Navier–Stokes equations.

Chapter 2

Scale Separation and Filtering

2.1 Scale Separation

To model the large-scale motion of a turbulent flow without computing the small-scale motion directly, we need to separate each of the flow quantities $\mathbf{u}$ and p into a large-scale part and a small-scale fluctuation. This is achieved by taking averages, denoted by $\langle \cdot \rangle$, of the quantities and defining the fluctuations as the differences from these averages:

$$\mathbf{u} = \langle \mathbf{u} \rangle + \mathbf{u}', \qquad p = \langle p \rangle + p'. \tag{2.1}$$

Conventional turbulence models, which use the Reynolds Averaged Navier–Stokes (RANS) approach, use the long-time average introduced by Reynolds (1895)

$$\langle \mathbf{u} \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T \mathbf{u} \, \mathrm{d}t, \qquad \langle p \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T p \, \mathrm{d}t, \tag{2.2}$$

to separate out the large scales. However, as Berselli *et al.* (2006) point out, this average erases all time dependence, so dynamic features of the flow outside statistical steady states cannot be captured.

To combat this problem, LES uses a local spatial average, which preserves these dynamic features, but still acts as a filter to isolate the large scales. According to Sagaut (2006), the averaging operator $\langle \cdot \rangle$ must satisfy the following properties so that we can manipulate the Navier–Stokes equations after applying the filter:

1. Preservation of constants

$$\langle a \rangle = a, \quad \text{for } a = \text{constant}. \tag{2.3}$$

2. Linearity

$$\langle a\phi + b\psi \rangle = a\langle \phi \rangle + b\langle \psi \rangle, \qquad \text{for } a, b \text{ constant}. \tag{2.4}$$

3. Commutation with differentiation

$$\left\langle \frac{\partial \phi}{\partial s} \right\rangle = \frac{\partial \langle \phi \rangle}{\partial s}, \qquad \text{for } s \in \{x_1, x_2, x_3, t\}. \tag{2.5}$$

Applying a filter to the NSEs, and using these three properties leads to the Space Filtered Navier–Stokes Equations:

$$\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \nabla \cdot \langle \mathbf{u}\mathbf{u} \rangle = -\nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{u} \rangle + \langle \mathbf{F} \rangle, \tag{2.6}$$

$$\nabla \cdot \langle \mathbf{u} \rangle = 0. \tag{2.7}$$

The closure problem for LES arises from the nonlinear term in the filtered momentum equation (2.6), since $\langle \mathbf{u}\mathbf{u} \rangle \neq \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle$. This is the same issue that needs to be overcome when modelling multiphase flow, where averages are taken over the different phases within a control volume. We will return to this problem after introducing some concrete filters.

2.2 Example Filters

A good way to ensure the commutation with spatial differentiation property (2.5) holds is to represent the filter mathematically by a convolution with a filter kernel G:

$$\langle \mathbf{u} \rangle (\mathbf{x}, t) = (G * \mathbf{u})(\mathbf{x}, t) = \int_{\mathbb{R}^3} G(\mathbf{x} - \boldsymbol{\xi}) \mathbf{u}(\boldsymbol{\xi}, t) \, \mathrm{d}\boldsymbol{\xi}. \tag{2.8}$$

Since linearity is a fundamental property of the convolution, this definition ensures linearity of the filter independently of the choice of G. To satisfy the constant preservation property (2.3), we must also have

$$\int_{\mathbb{R}^3} G(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} = 1. \tag{2.9}$$

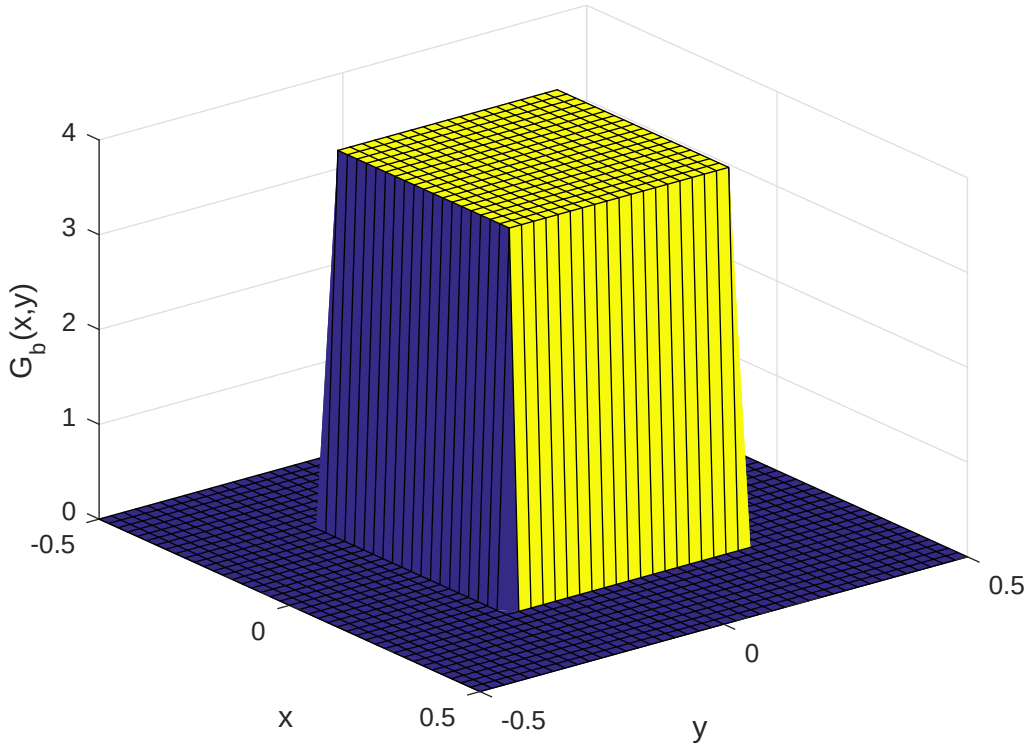

Figure 2.1: Two-dimensional representation of the box kernel with $\Delta = 0.5$.

There are three filters in particular which are most commonly used in Large Eddy Simulation. In the following definitions, Δ is the cutoff length scale, which is used as the mesh spacing in a numerical simulation. Features of the flow smaller than this length scale will be neglected by the filter, so these must be modelled by extra terms (see section 2.3). The definitions given in this section are 3-D generalisations of the 1-D filter definitions used by Sagaut (2006).

The first of the filters is the 'box filter', which is a simple implementation of the idea of a local, spatial average. Its kernel is

$$G_b(\mathbf{x}) = \begin{cases} \frac{1}{\Delta^3} & \text{if } |x_i| \leq \frac{\Delta}{2} \quad \text{for all } i \in \{1,2,3\}, \\ 0 & \text{otherwise,} \end{cases} \tag{2.10}$$

as shown in Figure 2.1.

Another is the 'spectral cutoff filter', which is a direct implementation of the idea of filtering out small spatial scales. If we define the Fourier transform $\widehat{F}$ of a function F as

$$\widehat{F}(\mathbf{k},t) = \int_{\mathbb{R}^3} F(\mathbf{x},t) e^{-i\mathbf{k}\cdot\mathbf{x}} \, \mathrm{d}\mathbf{x}, \tag{2.11}$$

a standard convolution result tells us that

$$\widehat{\langle\phi\rangle} = \widehat{G}\widehat{\phi}. \tag{2.12}$$

We can think of the values of $\widehat{\phi}$ at small wavenumbers $k = |\mathbf{k}|$ as the contribution of ϕ at large scales and vice versa. Therefore, it makes sense to first define the spectral cutoff

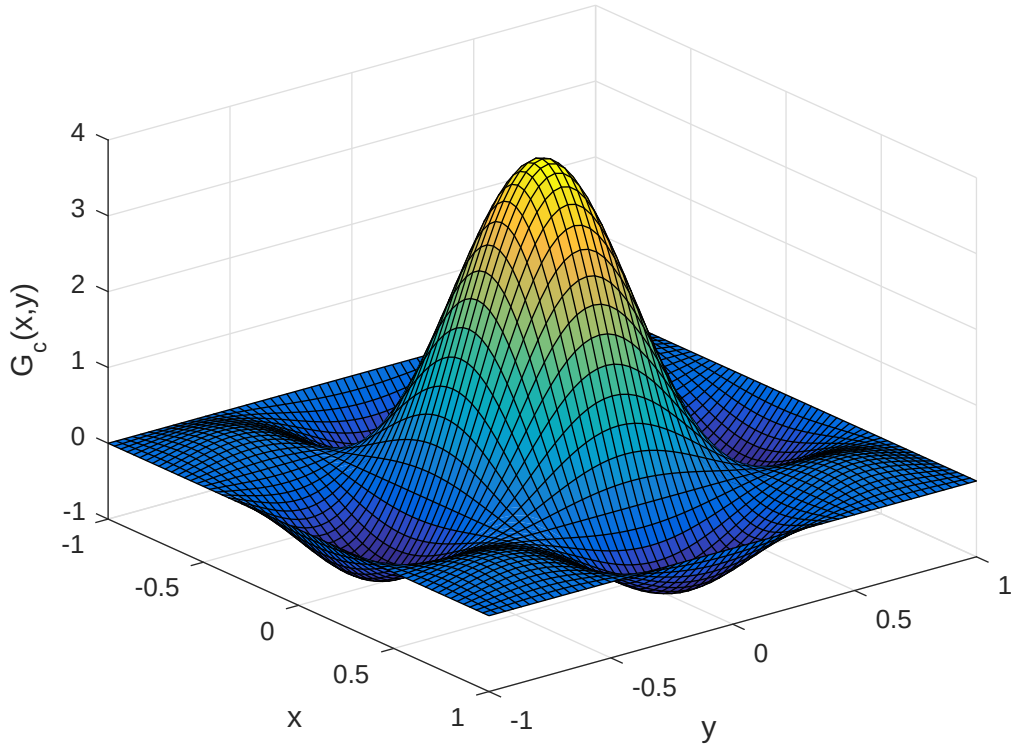

Figure 2.2: Two-dimensional representation of the spectral cutoff kernel with $\Delta = 0.5$.

filter in terms of the Fourier transform of its kernel:

$$\widehat{G_c}(\mathbf{k}) = \begin{cases} 1 & \text{if } |k_i| \leq k_c \quad \text{for all } i \in \{1,2,3\}, \\ 0 & \text{otherwise,} \end{cases} \tag{2.13}$$

where $k_c = \pi/\Delta$. By inverting the transform, we obtain the spectral cutoff filter kernel in physical space, as shown in Figure 2.2:

$$G_c(\mathbf{x}) = \frac{\sin(\frac{\pi x_1}{\Delta})\sin(\frac{\pi x_2}{\Delta})\sin(\frac{\pi x_3}{\Delta})}{\pi^3 x_1 x_2 x_3}. \tag{2.14}$$

The third commonly used filter takes a similar form under a Fourier transform as it does in physical space. Thus, it is a good example of both a local spatial average and a large-scale filter. This filter has a Gaussian as its kernel, as shown in Figure 2.3:

$$G_g(\mathbf{x}) = \left(\frac{\gamma}{\pi}\right)^{3/2} \frac{1}{\Delta^3} \exp\left(-\frac{\gamma\,|\mathbf{x}|^2}{\Delta^2}\right), \tag{2.15}$$

where the parameter γ sets the width of the Gaussian relative to the cutoff scale Δ. In LES, γ is usually set to be 6 (Berselli *et al.*, 2006).

The Gaussian and the spectral cutoff filter kernel are both non-local in physical space. However, the fast decay away from $\mathbf{x} = \mathbf{0}$ in both G_g and G_c suggest that this will not cause issues in simulations except near boundaries. We also note that the spectral cutoff filter kernel is negative in half the domain, which will have certain implications later in section 3.3.

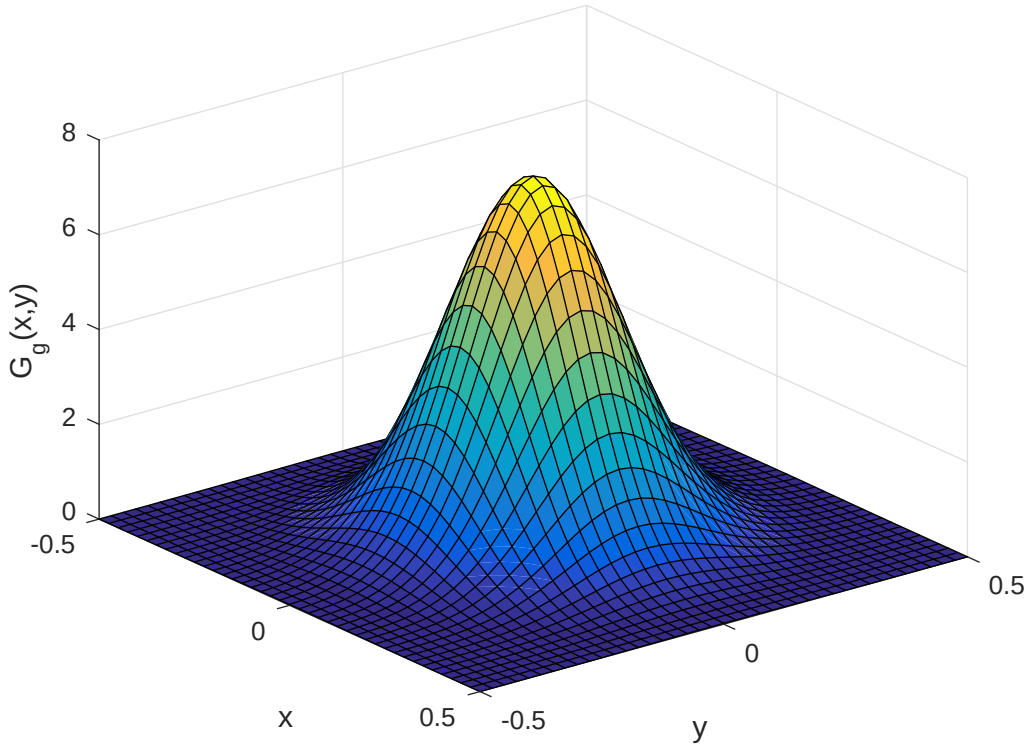

Figure 2.3: Two-dimensional representation of the Gaussian kernel with $\Delta = 0.5$.

2.2.1 Differential Filters

In some cases, the filter kernel used in LES can usefully be thought of as a Green's function for a linear differential operator. Germano (1986) first proposed using this type of filter, which allows the original variables to be written in terms of the filtered variables as

$$\phi = \mathcal{L}(\langle\phi\rangle), \tag{2.16}$$

where $\mathcal{L}$ is a differential operator which has the filter kernel G as its Green's function. Following Sagaut (2006), we can Taylor expand

$$\phi = \langle\phi\rangle + \alpha_i \frac{\partial\langle\phi\rangle}{\partial x_i} + \alpha_{ij}\frac{\partial^2\langle\phi\rangle}{\partial x_i \partial x_j} + ... \tag{2.17}$$

where α_i, α_{ij}, *etc.* are scaling parameters. In (2.17), and throughout this dissertation, we make use of Einstein's summation convention unless explicitly stated otherwise. We will use α to denote our cutoff length scale in this subsection (rather than Δ) to avoid confusion with differential operators. Differential filters are classified by their corresponding inverse operator, i.e. an elliptic filter uses the Green's function for an elliptic operator.

Berselli *et al.* (2006) suggested that differential filters are a more natural fit for bounded domains than the original convolution definition of a filter. Since almost all practical applications of turbulence modelling involve boundaries, differential filters may well become more widely used in future developments of LES.

The most commonly used differential filter is based on the modified Helmholtz operator, $\mathcal{L} = I - \alpha^2\nabla^2$, so we can define the filter implicitly by

$$\phi = \mathcal{L}(\langle\phi\rangle) = \langle\phi\rangle - \alpha^2\nabla^2\langle\phi\rangle. \tag{2.18}$$

Inverting this operator using its free-space Green's function defines a convolution filter:

$$\langle\phi\rangle = \frac{1}{4\pi\alpha^2}\int_{\mathbb{R}^3}\frac{\phi(\boldsymbol{\xi},t)}{|\mathbf{x}-\boldsymbol{\xi}|}\exp\left(-\frac{|\mathbf{x}-\boldsymbol{\xi}|}{\alpha}\right)\,\mathrm{d}\boldsymbol{\xi}, \tag{2.19}$$

but (2.18) can also be used in domains with boundaries, for which the equivalent convolution filter (2.19) would use the Green's function for such domains. Equation (2.18) differs from the regular Helmholtz operator [$\mathcal{L} = I + \alpha^2\nabla^2$] to ensure the normalizability property, otherwise the exponent in the convolution expression would be positive. Also, the Fourier transform of (2.18) is given by

$$\hat{\phi} = (1 + \alpha^2 k^2)\langle\hat{\phi}\rangle, \tag{2.20}$$

with a positive definite prefactor, so the operator is always invertible. Again, this does not hold for the regular Helmholtz operator.

2.3 Space Filtered Navier–Stokes Equations

As mentioned before, the nonlinear term $\langle \mathbf{uu} \rangle$ gives us a closure problem for the filtered equations. To gain insight into what a good closure model would involve, we will now explore how to decompose the nonlinear term. Using the relation for $\mathbf{u}$ from (2.1),

$$\langle \mathbf{uu} \rangle = \langle (\langle \mathbf{u} \rangle + \mathbf{u}')(\langle \mathbf{u} \rangle + \mathbf{u}') \rangle, \tag{2.21}$$

which, using the linearity property of filtering, leads to

$$\langle \mathbf{uu} \rangle = \langle \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle \rangle + \langle \mathbf{u}' \langle \mathbf{u} \rangle \rangle + \langle \langle \mathbf{u} \rangle \mathbf{u}' \rangle + \langle \mathbf{u}' \mathbf{u}' \rangle. \tag{2.22}$$

We can now rewrite (2.6) as

$$\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \nabla \cdot \langle \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle \rangle = -\nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{u} \rangle + \langle \mathbf{F} \rangle - \nabla \cdot \mathbf{T}, \tag{2.23}$$

where the tensor $\mathbf{T}$ consists of the last three terms of (2.22). These terms can also be expressed as a sum of two tensors: the cross-stress tensor $\mathbf{C}$, which represents the interaction of the small scale motion with the larger scales, and the Reynolds stress tensor $\mathbf{R}$, which accounts for the interactions between subgrid scales (Sagaut, 2006). Their components are given by

$$C_{ij} = \langle u_i' \langle u_j \rangle \rangle + \langle \langle u_i \rangle u_j' \rangle, \tag{2.24}$$

$$R_{ij} = \langle u_i' u_j' \rangle. \tag{2.25}$$

2.3.1 Key Differences Between LES and RANS

An averaging operator is called a Reynolds operator if, in addition to the properties already listed in section 2.1, it also satisfies

$$\langle \langle \phi \rangle \psi \rangle = \langle \phi \rangle \langle \psi \rangle \quad \text{for all } \phi, \psi. \tag{2.26}$$

Using linearity and preservation of constants, this also implies

$$\langle \langle \phi \rangle \rangle = \langle \phi \rangle \quad \text{for all } \phi. \tag{2.27}$$

This second property is clearly not satisfied by a general convolution filter.

However, for the long-time average (2.2) used in RANS, the time dependence of the flow quantities is removed by applying the average once. Property (2.26) is then satisfied, so the long-time average is a Reynolds operator:

$$\langle \langle \phi \rangle \psi \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T \langle \phi \rangle(\mathbf{x}) \psi(\mathbf{x}, t) \, \mathrm{d}t, \tag{2.28a}$$

$$= \langle \phi \rangle \lim_{T \to \infty} \frac{1}{T} \int_0^T \psi \, \mathrm{d}t = \langle \phi \rangle \langle \psi \rangle. \tag{2.28b}$$

In particular, a Reynolds operator produces the following results for terms in the averaged NSEs:

$$\langle \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle \rangle = \langle \mathbf{u} \rangle \langle \langle \mathbf{u} \rangle \rangle \;\Rightarrow\; \langle \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle \rangle = \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle, \tag{2.29a}$$

$$\langle \mathbf{u}' \rangle = \langle \mathbf{u} - \langle \mathbf{u} \rangle \rangle = \langle \mathbf{u} \rangle - \langle \langle \mathbf{u} \rangle \rangle \;\Rightarrow\; \langle \mathbf{u}' \rangle = \mathbf{0}, \tag{2.29b}$$

$$\mathbf{C} = \langle \mathbf{u}' \langle \mathbf{u} \rangle \rangle + \langle \langle \mathbf{u} \rangle \mathbf{u}' \rangle = \langle \mathbf{u}' \rangle \langle \mathbf{u} \rangle + \langle \mathbf{u} \rangle \langle \mathbf{u}' \rangle \;\Rightarrow\; \mathbf{C} = \mathbf{0}. \tag{2.29c}$$

Applying these to momentum equation (2.23), we obtain the Reynolds Averaged Navier–Stokes momentum equation:

$$\nabla \cdot (\langle \mathbf{u} \rangle \langle \mathbf{u} \rangle) = -\nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{u} \rangle + \langle \mathbf{F} \rangle - \nabla \cdot \mathbf{R}. \tag{2.30}$$

Here, the only term not expressed in terms of the filtered variables is the Reynolds stress $\mathbf{R} = \langle \mathbf{u}'\mathbf{u}' \rangle$, so this is the only term requiring a closure model. Helpfully, it is obvious from the definition that $\mathbf{R}$ is a symmetric tensor, and it can also be shown that the Reynolds stress is positive semidefinite (see section 3.3).

Since the convolution filters used in LES are not Reynolds operators, none of the above results apply directly to the spatially-averaged equations. Analogies between LES and RANS can only be reliably drawn if certain restrictions are imposed on the extra terms that arise in the spatially-averaged equations. The implications of some of these restrictions will be explored in Chapter 3.

2.3.2 Leonard Decomposition

For a filter that is not a Reynolds operator, evaluating the $\nabla \cdot \langle \langle \mathbf{u} \rangle \langle \mathbf{u} \rangle \rangle$ term in the momentum equation (2.23) requires a second application of the filter. Leonard (1974) therefore proposed a further decomposition of the nonlinear term, introducing the subgrid-scale stress tensor as

$$\tau_{ij} = \langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle = L_{ij} + C_{ij} + R_{ij}, \tag{2.31}$$

where the Leonard stress tensor is

$$L_{ij} = \langle \langle u_i \rangle \langle u_j \rangle \rangle - \langle u_i \rangle \langle u_j \rangle. \tag{2.32}$$

The momentum equation (2.6) now becomes

$$\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{u} \rangle \langle \mathbf{u} \rangle) = -\nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{u} \rangle + \langle \mathbf{F} \rangle - \nabla \cdot \boldsymbol{\tau}. \tag{2.33}$$

We must now find an appropriate closure model for $\boldsymbol{\tau}$ in terms of the filtered variables, so that the above differential equation, and the filtered mass conservation equation (2.7), can be discretized and solved numerically.

Chapter 3

Physical Constraints for Subgrid-Scale Models

Analysis of the Navier–Stokes equations shows that they satisfy various properties corresponding to physical laws and symmetries. In this chapter, we will describe a number of these properties, and analyse the filtered NSEs to derive a number of constraints on the turbulence model. These constraints ensure that the model remains consistent with underlying qualitative properties of the fluid flow.

3.1 Galilean Invariance

The Navier–Stokes equations are known to be invariant under the Galilean group of transformations, which is generated by 'Galilean boosts'

$$\mathbf{x}^* = \mathbf{x} + \mathbf{V}t + \mathbf{b}, \qquad t^* = t, \tag{3.1}$$

as well as constant rotations

$$\mathbf{x}^* = A\mathbf{x}, \qquad t^* = t, \tag{3.2}$$

and time translations

$$\mathbf{x}^* = \mathbf{x}, \qquad t^* = t + s. \tag{3.3}$$

Here, $\mathbf{V}$ and $\mathbf{b}$ are constant vectors, $A \in O(3)$ is a constant 3×3 orthogonal matrix, and s is a constant scalar.

We now want to show that the filtered NSEs are also Galilean invariant. Following the approach of Speziale (1985*a*), it is only necessary to show that the filtered part of a Galilean invariant function is also Galilean invariant. Starting with the Galilean boosts from (3.1), let ϕ be such a function, with its transformation ϕ^* defined by

$$\phi^*(\mathbf{x}^*, t^*) = \phi(\mathbf{x}, t). \tag{3.4}$$

We then consider the Galilean transformation of the filtered part of ϕ, as given by

$$\langle\phi\rangle^*(\mathbf{x}^*, t^*) = \int_D G(\mathbf{x}^* - \boldsymbol{\xi}^*)\phi^*(\boldsymbol{\xi}^*, t^*)\,\mathrm{d}\boldsymbol{\xi}^*, \tag{3.5}$$

where G is a normalised filter function as in Chapter 2. The change of variables (3.1) implies

$$\mathbf{x}^* - \boldsymbol{\xi}^* = \mathbf{x} + \mathbf{V}t + \mathbf{b} - (\boldsymbol{\xi} + \mathbf{V}t + \mathbf{b}) = \mathbf{x} - \boldsymbol{\xi}, \tag{3.6}$$

and

$$\mathrm{d}\boldsymbol{\xi}^* = \left|\frac{\partial \xi_i^*}{\partial \xi_j}\right| \mathrm{d}\boldsymbol{\xi}, \tag{3.7}$$

where $|\partial \xi_i^*/\partial \xi_j|$ is the Jacobian of the transformation (3.1). This determinant is equal to 1 for all transformations in the Galilean group, so substituting (3.4), (3.6) and (3.7) into (3.5) gives the desired result

$$\langle\phi\rangle^*(\mathbf{x}^*, t^*) = \int_D G(\mathbf{x} - \boldsymbol{\xi})\phi(\boldsymbol{\xi}, t)\,\mathrm{d}\boldsymbol{\xi} \equiv \langle\phi\rangle(\mathbf{x}, t). \tag{3.8}$$

Since time translations (3.3) produce no change of spatial variable, the above proof becomes trivial, as (3.6) and (3.7) are satisfied automatically. However, in the case of the constant rotation (3.2), relation (3.6) is not satisfied. Therefore, the above result only holds if the filter function G satisfies

$$G(A\mathbf{x}) = G(\mathbf{x}) \quad \text{for all } A \in O(3), \qquad \text{i.e. } G(\mathbf{x}) = \tilde{G}(|\mathbf{x}|). \tag{3.9}$$

for some function $\tilde{G}$. Hence, we should impose that the filter function is spherically symmetric,[1] in which case the filtered equations are Galilean invariant.

We must note, however, that differentiating the transformation (3.1) gives

$$\mathbf{u}^* = \frac{D\mathbf{x}^*}{Dt^*} = \frac{D}{Dt}(\mathbf{x} + \mathbf{V}t + \mathbf{b}) = \mathbf{u} + \mathbf{V}. \tag{3.10}$$

Although this shows that $\mathbf{u}$ is not strictly invariant under the transformation, it is consistent with the notion of Galilean invariance (or covariance) in particle mechanics. Following the above proof with $\mathbf{u}$ replacing ϕ, we obtain the result

$$\langle\mathbf{u}\rangle^* = \langle\mathbf{u}\rangle + \mathbf{V}, \tag{3.11}$$

which combined with (3.10) also tells us that the fluctuation $\mathbf{u}' = \mathbf{u} - \langle\mathbf{u}\rangle$ satisfies

$$\mathbf{u}'^* = \mathbf{u}', \qquad \langle\mathbf{u}'^*\rangle = \langle\mathbf{u}'\rangle. \tag{3.12}$$

We can directly apply these results to the definition of $\boldsymbol{\tau}$ (see (2.31) in the previous chapter) to investigate how it transforms under a Galilean boost:

$$\begin{aligned}
\boldsymbol{\tau}^* &= \langle\mathbf{u}^*\mathbf{u}^*\rangle - \langle\mathbf{u}^*\rangle\langle\mathbf{u}^*\rangle, && \text{(3.13a)}\\
&= \langle(\mathbf{u} + \mathbf{V})(\mathbf{u} + \mathbf{V})\rangle - \langle\mathbf{u} + \mathbf{V}\rangle\langle\mathbf{u} + \mathbf{V}\rangle, && \text{(3.13b)}\\
&= \langle\mathbf{u}\mathbf{u}\rangle - \langle\mathbf{u}\rangle\langle\mathbf{u}\rangle. && \text{(3.13c)}
\end{aligned}$$

This shows that $\boldsymbol{\tau}$ is invariant under Galilean boosts, so a physically reasonable closure model should exhibit this property.

Many subgrid models make use of the Leonard (1974) decomposition of the subgrid-scale stress tensor, which we introduced in section 2.3.2:

$$\begin{aligned}
\tau_{ij} &= L_{ij} + C_{ij} + R_{ij}, && \text{(3.14a)}\\
L_{ij} &= \langle\langle u_i\rangle\langle u_j\rangle\rangle - \langle u_i\rangle\langle u_j\rangle, && \text{(3.14b)}\\
C_{ij} &= \langle\langle u_i\rangle u_j'\rangle + \langle u_i'\langle u_j\rangle\rangle, && \text{(3.14c)}\\
R_{ij} &= \langle u_i' u_j'\rangle. && \text{(3.14d)}
\end{aligned}$$

[1] Ghosal (1999) notes that this is not always necessary in practical implementations, since on a coarse grid there will be a large number of eddies at a smaller scale than Δ. This will cause the filtered variables to be almost independent of the shape of the filter, in the same way that the specific heat of an object does not depend on the shape of the object if its dimensions are much larger than the molecular scale.

Since L_{ij} can be calculated directly, the problem can be reduced to finding a closure model for C_{ij} and R_{ij}. However, Speziale (1985*a*) noted that, although τ_{ij} is invariant under the transformation (3.1), its constituent parts transform as

$$L^*_{ij} = L_{ij} - V_i\langle u'_j\rangle - V_j\langle u'_i\rangle, \tag{3.15a}$$
$$C^*_{ij} = C_{ij} + V_i\langle u'_j\rangle + V_j\langle u'_i\rangle, \tag{3.15b}$$
$$R^*_{ij} = R_{ij}, \tag{3.15c}$$

as found by applying (3.10) to (3.12) to the definitions of these tensors. This shows that R_{ij} and the sum $L_{ij} + C_{ij}$ are Galilean invariant, but the individual tensors L_{ij} and C_{ij} are not. In models that calculate L_{ij} explicitly, the modelled cross-stresses C_{ij} must have a Galilean dependence as above.

If we take the filter to be spherically symmetric, as suggested by our earlier result, then taking the same approach as before but with constant rotations (3.2) gives

$$\mathbf{u}^* = A\mathbf{u}, \qquad \langle\mathbf{u}\rangle^* = A\langle\mathbf{u}\rangle, \qquad \mathbf{u}'^* = A\mathbf{u}'. \tag{3.16}$$

Inserting these expressions into $\boldsymbol{\tau}$ gives

$$\tau^*_{ij} = A_{ik}A_{jl}\tau_{kl}, \qquad \text{i.e. } \boldsymbol{\tau}^* = A\boldsymbol{\tau}A^T. \tag{3.17}$$

Analogous results can be found for the other tensors L_{ij}, C_{ij}, and R_{ij} due to linearity of the filtering operation. Therefore all of the subgrid tensors transform correctly as second-rank tensors (i.e. are covariant) under rotations.

3.2 Generalized Central Moments and Averaging Invariance

In section 2.3.1, we showed that using a Reynolds operator for the average gives a simpler form for the subgrid tensor in the filtered NSEs. Using the properties of a Reynolds operator $\langle\cdot\rangle_R$ and some simple algebra, we get the following relations for the central moments $\langle u'_i u'_j\rangle_R$ and $\langle u'_i u'_j u'_k\rangle_R$:

$$\langle u'_i u'_j\rangle_R = \langle u_i u_j\rangle_R - \langle u_i\rangle_R\langle u_j\rangle_R, \tag{3.18}$$
$$\begin{aligned}\langle u'_i u'_j u'_k\rangle_R =& \langle u_i u_j u_k\rangle_R - \langle u_i\rangle_R\langle u'_j u'_k\rangle_R - \langle u_j\rangle_R\langle u'_k u'_i\rangle_R \\ &- \langle u_k\rangle_R\langle u'_i u'_j\rangle_R - \langle u_i\rangle_R\langle u_j\rangle_R\langle u_k\rangle_R.\end{aligned} \tag{3.19}$$

Germano (1992) explained that in statistical turbulence modelling, these relations are used to derive evolution equations for the central moments. However, trying to do this for a non-Reynolds averaging operator $\langle\cdot\rangle$ results in a much more complicated system. Instead of writing out long expressions for these moments, Germano (1992) proposed that we formally define a set of generalised central moments that satisfy equivalent relations to those above:

$$\tau(u_i, u_j) = \langle u_i u_j\rangle - \langle u_i\rangle\langle u_j\rangle, \tag{3.20}$$
$$\begin{aligned}\tau(u_i, u_j, u_k) =& \langle u_i u_j u_k\rangle - \langle u_i\rangle\tau(u_j, u_k) - \langle u_j\rangle\tau(u_k, u_i) \\ &- \langle u_k\rangle\tau(u_i, u_j) - \langle u_i\rangle\langle u_j\rangle\langle u_k\rangle.\end{aligned} \tag{3.21}$$

We define $\tau(u_i, u_j)$ to be the same as the subgrid-scale stress tensor τ_{ij} that we defined previously. From the relations (3.20) and (3.21), we can see that it is best to work in index notation for manipulating the generalised central moments. We write the i^{th} component of the Navier–Stokes momentum equation as

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_k}\left(u_i u_k\right) = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_k \partial x_k} + F_i. \tag{3.22}$$

By multiplying this equation by u_j, and adding it to the same equation with the indices i and j switched, we obtain the equation[2]

$$\begin{aligned}\frac{\partial (u_i u_j)}{\partial t} + \frac{\partial}{\partial x_k}\left(u_i u_j u_k\right) = &- \frac{\partial}{\partial x_k}\left[p u_i \delta_{jk} + p u_j \delta_{ik} - \nu \frac{\partial (u_i u_j)}{\partial x_k}\right] + 2 p s_{ij} \\ &- 2\nu \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k} + u_i F_j + u_j F_i,\end{aligned} \tag{3.23}$$

where $s_{ij} = \dfrac{1}{2}\left(\dfrac{\partial u_i}{\partial x_j} + \dfrac{\partial u_j}{\partial x_i}\right)$ is the rate-of-strain tensor. We can now use this relation to derive a further equation involving the generalised central moments. By applying the filtering operation to (3.23), deriving a similar relation from the filtered NSEs, and performing some further algebra, we obtain

$$\begin{aligned}\frac{\partial \tau(u_i, u_j)}{\partial t} + \frac{\partial}{\partial x_k}\left(\tau(u_i, u_j)\langle u_k \rangle\right) = &- \frac{\partial}{\partial x_k}\Big\{ \tau(u_i, u_j, u_k) + \tau(p, u_i)\delta_{jk} \\ &+ \tau(p, u_j)\delta_{ik} - \nu \frac{\partial \tau(u_i, u_j)}{\partial x_k}\Big\} \\ &+ 2\tau(p, s_{ij}) - 2\nu\tau\left(\frac{\partial u_i}{\partial x_k}, \frac{\partial u_j}{\partial x_k}\right) \\ &- \tau(u_i, u_k)\frac{\partial \langle u_j \rangle}{\partial x_k} - \tau(u_j, u_k)\frac{\partial \langle u_i \rangle}{\partial x_k} \\ &+ \tau(u_i, F_j) + \tau(u_j, F_i).\end{aligned} \tag{3.24}$$

This equation governs the evolution of the generalised central moments, and the key idea to take away from it is that this relation does not depend on the filter operation. This property is referred to as "averaging invariance" by Germano (1992), and it allows us to derive extra relations to use in modelling turbulent flow.

For example, if we follow Germano (1992) in defining the generalised turbulent kinetic energy density as

$$E_T = \frac{1}{2}\tau(u_i, u_i), \tag{3.25}$$

and then contract relation (3.24) with δ_{ij}, we obtain an evolution equation for the turbulent kinetic energy density:

$$\begin{aligned}\frac{\partial E_T}{\partial t} + \frac{\partial (E_T \langle u_k \rangle)}{\partial x_k} = &- \frac{\partial}{\partial x_k}\left[\frac{1}{2}\tau(u_i, u_i, u_k) + \tau(p, u_k) - \nu \frac{\partial E_T}{\partial x_k}\right] \\ &- \nu\tau\left(\frac{\partial u_i}{\partial x_k}, \frac{\partial u_i}{\partial x_k}\right) - \tau(u_i, u_k)\langle s_{ik} \rangle + \tau(u_i, F_i).\end{aligned} \tag{3.26}$$

[2]We give a full derivation of equations (3.23), (3.24) & (3.26) in Appendix A.

We can also use the generalised central moments to construct another decomposition of the subgrid-scale stress tensor. In the spirit of the previously mentioned Leonard (1974) decomposition, Germano (1992) proposed that the generalised second central moment (i.e. the subgrid-scale stress tensor) can be decomposed purely in terms of generalised central moments of the mean velocity and the fluctuation:

$$\tau(u_i, u_j) = \mathcal{L}_{ij} + \mathcal{C}_{ij} + \mathcal{R}_{ij}, \tag{3.27}$$

where

$$\mathcal{L}_{ij} = \tau(\langle u_i \rangle, \langle u_j \rangle), \tag{3.28a}$$
$$\mathcal{C}_{ij} = \tau(\langle u_i \rangle, u'_j) + \tau(u'_i, \langle u_j \rangle), \tag{3.28b}$$
$$\mathcal{R}_{ij} = \tau(u'_i, u'_j). \tag{3.28c}$$

We can use the results of section 3.1 to analyse the properties of the new tensors in this decomposition. In particular, $\tau_{ij} = \tau(u_i, u_j)$ was shown to be invariant under Galilean transformations, so we know that $\mathcal{L}_{ij}$ will be Galilean invariant since $\langle \mathbf{u} \rangle$ transforms in the same way as $\mathbf{u}$ (see (3.11) or (3.16)). The new Reynolds stress $\mathcal{R}_{ij}$ will also be Galilean invariant, since $\mathbf{u}'$ is invariant under Galilean boosts and transforms as $\mathbf{u}$ does under rotations from (3.16). Since

$$\mathcal{C}_{ij} = \tau(u_i, u_j) - \mathcal{L}_{ij} - \mathcal{R}_{ij}, \tag{3.29}$$

consists solely of invariant terms, the new cross-stress tensor $\mathcal{C}_{ij}$ must also be Galilean invariant. With this decomposition, we can impose Galilean invariance on any proposed closure model, even when the resolved stresses $\mathcal{L}_{ij}$ are modelled separately.

3.3 Realizability Conditions

Vreman *et al.* (1994) give the following three conditions for a tensor $\mathbf{T}$ to be positive semidefinite:

$$T_{ii} \geq 0, \qquad \text{for} \quad i \in \{1, 2, 3\}, \tag{3.30}$$
$$|T_{ij}| \leq \sqrt{T_{ii} T_{jj}}, \qquad \text{for} \quad i, j \in \{1, 2, 3\}, \tag{3.31}$$
$$\det \mathbf{T} \geq 0. \tag{3.32}$$

Schumann (1977) was the first to observe that the Reynolds stress tensor R_{ij} should satisfy these conditions, i.e. when using a statistical average in turbulence modelling, the subgrid-scale stress tensor must be positive semidefinite. We will refer to equations (3.30) to (3.32) as the 'realizability conditions' from now on. These are the properties one would expect from a tensor of the form $\langle u'_i u'_j \rangle$ since it is constructed from the average of a tensor product of a vector with itself.

As usual, things are not so simple when $\langle \cdot \rangle$ is not a Reynolds operator. Instead of trying to derive similar conditions for the subgrid-scale tensor $\boldsymbol{\tau}$ from the filtered equations, we will investigate the implications of imposing the realizability conditions on $\boldsymbol{\tau}$. Vreman *et al.* (1994) suggested that ensuring the positivity of the generalised turbulent kinetic energy (3.25) provides one justification for imposing these conditions. For example, models that use E_T to correspond with the physical notion of kinetic energy

may become ill-defined if a negative value arises. If $\boldsymbol{\tau}$ is positive semidefinite, we also obtain the following upper bound directly from (3.31):

$$|\tau_{ij}| \leq 2E_T \quad \text{for all } i, j. \tag{3.33}$$

We will now follow the approach of Vreman *et al.* (1994) to prove that $\boldsymbol{\tau}$ is positive semidefinite if and only if the filter function G is non-negative. Firstly, suppose $G \geq 0$ everywhere. For each $\mathbf{x}$ in the domain D, we define a subset $S_{\mathbf{x}}$ as the support of the function $\boldsymbol{\xi} \mapsto G(\mathbf{x} - \boldsymbol{\xi})$, i.e. the closure of the set of $\boldsymbol{\xi}$ such that $G(\mathbf{x} - \boldsymbol{\xi})$ is non-zero. Let $F_{\mathbf{x}}$ be the space of real functions on this subset. Now, as $G \geq 0$ everywhere, we may define an inner product on $F_{\mathbf{x}}$ by

$$[f, g] = \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}, \qquad \text{for } f, g \in F_{\mathbf{x}}. \tag{3.34}$$

We use the definition of τ_{ij} and the preservation of constants property of the convolution with G to show that τ_{ij} can be expressed using this inner product:

$$\begin{aligned}
\tau_{ij} =& \langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle, && \text{(3.35a)}\\
=& \langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle - \langle u_j \rangle \langle u_i \rangle + \langle u_i \rangle \langle u_j \rangle, && \text{(3.35b)}\\
=& \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) u_i(\boldsymbol{\xi}) u_j(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} - \langle u_i \rangle(\mathbf{x}) \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) u_j(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} \\
& - \langle u_j \rangle(\mathbf{x}) \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) u_i(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} + \langle u_i \rangle(\mathbf{x}) \langle u_j \rangle(\mathbf{x}) \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}, && \text{(3.35c)}\\
=& \int_{S_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) (u_i(\boldsymbol{\xi}) - \langle u_i \rangle(\mathbf{x})) (u_j(\boldsymbol{\xi}) - \langle u_j \rangle(\mathbf{x})) \, \mathrm{d}\boldsymbol{\xi}, && \text{(3.35d)}\\
=& [u_i(\boldsymbol{\xi}) - \langle u_i \rangle(\mathbf{x}), u_j(\boldsymbol{\xi}) - \langle u_j \rangle(\mathbf{x})] \equiv [v_i^{\mathbf{x}}(\boldsymbol{\xi}), v_j^{\mathbf{x}}(\boldsymbol{\xi})], && \text{(3.35e)}
\end{aligned}$$

where we define

$$v_i^{\mathbf{x}}(\boldsymbol{\xi}) = u_i(\boldsymbol{\xi}) - \langle u_i \rangle(\mathbf{x}). \tag{3.36}$$

The final result (3.35e) says that τ_{ij} must take the form known as a Gramian matrix for each value of $\mathbf{x}$. Such a matrix is always positive semidefinite,[3] so the realizability conditions are satisfied.

Conversely, now suppose that $G(\mathbf{y}) < 0$ for some $\mathbf{y}$ in the domain D. If G is a continuous function, we can define the following neighbourhood of $\mathbf{y}$:

$$V = \{\boldsymbol{\eta} \in D : |\boldsymbol{\eta} - \mathbf{y}| < \delta\}, \tag{3.37}$$

where $\delta > 0$ is chosen such that $G(\boldsymbol{\eta}) < 0$ for all $\boldsymbol{\eta} \in V$. For each value of $\mathbf{x}$ we can also define the set $W_{\mathbf{x}}$ by

$$W_{\mathbf{x}} = \{\boldsymbol{\zeta} \in D : \mathbf{x} - \boldsymbol{\zeta} \in V\}. \tag{3.38}$$

Then, if we fix $\mathbf{x}$ and choose the function u_1 such that $u_1(\boldsymbol{\xi}) \neq 0$ if $\boldsymbol{\xi} \in W_{\mathbf{x}}$ and $u_1 = 0$ everywhere else, $\tau_{11}(\mathbf{x})$ must be negative:

$$\tau_{11}(\mathbf{x}) = \langle {u_1}^2 \rangle(\mathbf{x}) - (\langle u_1 \rangle(\mathbf{x}))^2 \leq \langle {u_1}^2 \rangle(\mathbf{x}) = \int_{W_{\mathbf{x}}} G(\mathbf{x} - \boldsymbol{\xi}) (u_1(\boldsymbol{\xi}))^2 \, \mathrm{d}\boldsymbol{\xi} < 0. \tag{3.39}$$

[3] See Appendix B for a proof.

This proves that if the filter is negative anywhere in the domain, then the subgrid tensor is not positive semidefinite. Hence $\boldsymbol{\tau}$ satisfies the realizability conditions (3.30) to (3.32) if and only if the function G in the convolution filter is non-negative.

Of the three most common filters, introduced in the previous chapter, only the spectral cutoff filter does not satisfy this positivity condition. Hence, this filter should not be used in conjunction with a formulation which models the generalised turbulent energy. However, this does not restrict use of the spectral cutoff filter in other LES models, where it may prove to be the most suitable.

3.4 Material Frame–Indifference

One of the most interesting analogies to make when thinking about turbulence modelling is between the subgrid-scale stresses and the elastic stresses inside non-Newtonian viscoelastic fluids. This was first suggested in a paper by Rivlin (1957) nearly 60 years ago, merely on the observation of secondary motions in the flows in both cases. Deville & Gatski (2012) provide a recent overview of the general principles involved in modelling the extra stresses for non-Newtonian fluids and warn that these stresses, although similar in some aspects to turbulent stresses (e.g. being second moments of a small-scale quantity), are fundamentally different. In particular, the viscoelastic stresses arise from the physical properties of the *fluid*, which typically contains suspended polymer molecules, whereas the turbulent stresses are purely related to the *flow* properties.

Nevertheless, it is interesting to investigate the possibility of similarities between these models. If the subgrid-scale stresses involved in LES share some mathematical or physical property with the viscoelastic stresses then an idea previously developed for modelling complex fluids could feasibly be adapted to improve the accuracy of a turbulence model or vice versa. One of the key methodological principles that is applied to the constitutive equations in any viscoelastic fluid model is Material Frame-Indifference (MFI), as proposed in Truesdell (1952) and Rivlin & Ericksen (1955). More work has been done on investigating MFI for conventional RANS turbulence models than for LES, but there are sources of interest for us to consider, in particular a paper by Speziale (1985*b*).

Speziale (1985*b*) follows a similar approach to that which we used earlier when investigating Galilean invariance. We now consider the more general Euclidean group of transformations, those for which

$$\mathbf{x}^* = Q(t)\mathbf{x} + \mathbf{b}(t), \quad t^* = t + a. \tag{3.40}$$

Here $Q(t)$ is any time-dependent orthogonal matrix, $\mathbf{b}(t)$ is any time-dependent vector and a is a constant. Rearranging this expression and differentiating with respect to time produces an equation for the velocity in the original frame in terms of the transformed variables:

$$\mathbf{x} = Q^T(\mathbf{x}^* - \mathbf{b}), \tag{3.41a}$$

$$\mathbf{u} = \dot{\mathbf{x}} = Q^T(\dot{\mathbf{x}^*} - \dot{\mathbf{b}}) + \dot{Q^T}(\mathbf{x}^* - \mathbf{b}), \tag{3.41b}$$

$$\mathbf{u} = Q^T\left[\dot{\mathbf{x}^*} - \dot{\mathbf{b}} - \dot{Q}Q^T(\mathbf{x}^* - \mathbf{b})\right]. \tag{3.41c}$$

To obtain the last line, we have used that Q is orthogonal. The matrix $\dot{Q}Q^T$ is thus anti-symmetric, so its action on a vector is equivalent to a wedge product with a vector

$-\boldsymbol{\Omega}(t)$, where $\boldsymbol{\Omega}(t)$ is the angular velocity of the transformed frame relative to the original frame (Woodhouse, 1987). Hence we can express $\mathbf{u}$ as

$$\mathbf{u} = Q^T \left[\mathbf{u}^* + \boldsymbol{\Omega}(t) \wedge (\mathbf{x}^* - \mathbf{b}(t)) - \dot{\mathbf{b}}(t) \right]. \tag{3.42}$$

To investigate whether the subgrid-scale stress tensor is invariant under a general change of frame, the above equation suggests that we must investigate how the filtered position vector $\langle \mathbf{x} \rangle$ transforms under (3.40). First, consider the filter acting on the position vector in the original frame:

$$\langle \mathbf{x} \rangle = \int_D G(\mathbf{x} - \boldsymbol{\xi}) \boldsymbol{\xi} \, \mathrm{d}\boldsymbol{\xi}. \tag{3.43}$$

Using the substitution $\boldsymbol{\xi} = \mathbf{x} - \mathbf{s}$, we can rewrite this integral as

$$\langle \mathbf{x} \rangle = \int_D G(\mathbf{s})(\mathbf{x} - \mathbf{s}) \, \mathrm{d}\mathbf{s}, \tag{3.44a}$$

$$= \mathbf{x} \int_D G(\mathbf{s}) \, \mathrm{d}\mathbf{s} - \int_D \mathbf{s} G(\mathbf{s}) \, \mathrm{d}\mathbf{s}. \tag{3.44b}$$

By the preservation of constants property for a filter, the first term of this expression is just $\mathbf{x}$. The second integral will disappear if the filter function G is an even function. This will happen if we enforce spherical symmetry of G (i.e. $G(\mathbf{s}) = \tilde{G}(|\mathbf{s}|)$) as suggested in section 3.1. Hence, the position vector $\mathbf{x}$ is unchanged by filtering. Since the filter operation is independent of time, position is also preserved in the transformed frame:

$$\langle \mathbf{x}^* \rangle = Q(t) \langle \mathbf{x} \rangle + \mathbf{b}(t) = Q(t)\mathbf{x} + \mathbf{b}(t) = \mathbf{x}^*. \tag{3.45}$$

We can now write down expressions for the filtered velocity $\langle \mathbf{u} \rangle$ and velocity fluctuation $\mathbf{u}'$:

$$\langle \mathbf{u} \rangle = Q^T \left[\langle \mathbf{u} \rangle^* + \boldsymbol{\Omega} \wedge \mathbf{x}^* - \dot{\mathbf{b}} \right], \tag{3.46a}$$

$$\mathbf{u}' = Q^T \mathbf{u}'^*. \tag{3.46b}$$

Since the velocity fluctuation is only affected by the orientation of the frame, the Reynolds stress tensor R_{ij} must transform as a second-rank tensor under a rotation:

$$u_i' = Q_{ki} u_k'^*, \qquad\qquad u_i' u_j' = Q_{ki} u_k'^* u_l'^* Q_{lj}, \tag{3.47}$$

which implies

$$\mathbf{R} = Q^T \mathbf{R}^* Q. \tag{3.48}$$

This is promising, but if we insert expression (3.46a) for the filtered velocity into the definition of the subgrid-scale stress tensor (2.31) we get

$$\begin{aligned} Q\boldsymbol{\tau}Q^T = \; & \boldsymbol{\tau}^* - \langle (\boldsymbol{\Omega} \wedge \mathbf{x}^*)\mathbf{u}^* \rangle - \langle \mathbf{u}^* (\boldsymbol{\Omega} \wedge \mathbf{x}^*) \rangle + (\boldsymbol{\Omega} \wedge \mathbf{x}^*) \langle \mathbf{u} \rangle^* + \langle \mathbf{u} \rangle^* (\boldsymbol{\Omega} \wedge \mathbf{x}^*) \\ & + (\boldsymbol{\Omega} \wedge \mathbf{x}^*)(\boldsymbol{\Omega} \wedge \mathbf{x}^*) - \langle (\boldsymbol{\Omega} \wedge \mathbf{x}^*)(\boldsymbol{\Omega} \wedge \mathbf{x}^*) \rangle. \end{aligned} \tag{3.49}$$

The above equation seems problematic, and it means that we cannot constrain our choice of $\boldsymbol{\tau}$ by imposing frame-indifference on the tensor. However, this is not where our analysis of the filtered NSEs must stop for MFI. Speziale (1985*b*) showed that the divergence of

the stress tensor $\nabla \cdot \boldsymbol{\tau}$ is in fact invariant under these Euclidean transformations, and only $\nabla \cdot \boldsymbol{\tau}$ appears in the filtered NSEs.

To gain more insight on the situation in the transformed frame, it is useful to express the Navier–Stokes equations in terms of the transformed variables. By differentiating the expression for $\mathbf{u}$ from (3.41c), we can obtain a relation for the material derivative $\mathrm{D}\mathbf{u}/\mathrm{D}t$:

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \ddot{\mathbf{x}} = Q^T\ddot{\mathbf{x}^*} - 2Q^T\dot{Q}Q^T(\dot{\mathbf{x}^*} - \dot{\mathbf{b}}) - Q^T\ddot{\mathbf{b}} - \frac{\mathrm{d}}{\mathrm{d}t}\left(Q^T\dot{Q}Q^T\right)(\mathbf{x}^* - \mathbf{b}), \tag{3.50a}$$

$$= Q^T\left[\ddot{\mathbf{x}^*} + 2\boldsymbol{\Omega} \wedge (\dot{\mathbf{x}^*} - \dot{\mathbf{b}}) - \ddot{\mathbf{b}} + \boldsymbol{\Omega} \wedge (\boldsymbol{\Omega} \wedge (\mathbf{x}^* - \mathbf{b})) + \dot{\boldsymbol{\Omega}} \wedge (\mathbf{x}^* - \mathbf{b})\right]. \tag{3.50b}$$

Replacing $\dot{\mathbf{x}^*}$ with $\mathbf{u}^*$, we get an expression for the Lagrangian acceleration of a fluid element:

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = Q^T\left[\frac{\mathrm{D}\mathbf{u}^*}{\mathrm{D}t^*} + 2\boldsymbol{\Omega} \wedge (\mathbf{u}^* - \dot{\mathbf{b}}) - \ddot{\mathbf{b}} + \boldsymbol{\Omega} \wedge (\boldsymbol{\Omega} \wedge (\mathbf{x}^* - \mathbf{b})) + \dot{\boldsymbol{\Omega}} \wedge (\mathbf{x}^* - \mathbf{b})\right]. \tag{3.51}$$

We can identify the additional terms in (3.51):

- $2\boldsymbol{\Omega} \wedge (\mathbf{u}^* - \dot{\mathbf{b}})$ is the Coriolis force due to the frame rotation,
- $-\ddot{\mathbf{b}}$ is the linear acceleration of the new frame relative to the original frame,
- $\boldsymbol{\Omega} \wedge (\boldsymbol{\Omega} \wedge (\mathbf{x}^* - \mathbf{b}))$ is the relative centripetal acceleration,
- $\dot{\boldsymbol{\Omega}} \wedge (\mathbf{x}^* - \mathbf{b})$ is the Poincaré (or Euler) force due to the angular acceleration of the frame.

The pressure and viscous terms in the Navier–Stokes momentum equation will transform as

$$p(\mathbf{x}, t) = p^*(\mathbf{x}^*, t), \qquad \nabla = Q^T\nabla^*, \tag{3.52a}$$

$$\nabla p = Q^T\nabla^* p^*, \tag{3.52b}$$

and

$$\mathbf{u} = Q^T[\mathbf{u}^* + \boldsymbol{\Omega} \wedge \mathbf{x}^* - \dot{\mathbf{b}}], \qquad \nabla^2 = \nabla^{*2}, \tag{3.53a}$$

$$\nabla^2\mathbf{u} = Q^T\nabla^{*2}\mathbf{u}^*. \tag{3.53b}$$

Thus, we can write the momentum equation (pre-multiplied by Q) in the transformed variables as

$$\begin{aligned}\frac{\mathrm{D}\mathbf{u}^*}{\mathrm{D}t^*} = &-\nabla^* p^* + \nu\nabla^{*2}\mathbf{u}^* - 2\boldsymbol{\Omega} \wedge (\mathbf{u}^* - \dot{\mathbf{b}}) + \ddot{\mathbf{b}} \\ &- \boldsymbol{\Omega} \wedge (\boldsymbol{\Omega} \wedge (\mathbf{x}^* - \mathbf{b})) - \dot{\boldsymbol{\Omega}} \wedge (\mathbf{x}^* - \mathbf{b}) + Q\mathbf{F}.\end{aligned} \tag{3.54}$$

In the above equation, we have not yet dealt with how the body force transforms. If we consider how $\mathbf{F}$, the body force per unit mass, affects a single point by Newton's second law

$$\mathbf{F} = \ddot{\mathbf{x}}, \tag{3.55}$$

then the relation in (3.50a) gives the transformation

$$\mathbf{F} = Q^T\left[\mathbf{F}^* + 2\boldsymbol{\Omega} \wedge (\mathbf{u}^* - \dot{\mathbf{b}}) - \ddot{\mathbf{b}} + \boldsymbol{\Omega} \wedge (\boldsymbol{\Omega} \wedge (\mathbf{x}^* - \mathbf{b})) + \dot{\boldsymbol{\Omega}} \wedge (\mathbf{x}^* - \mathbf{b})\right], \tag{3.56}$$

where $\mathbf{F}^*$ is the effective body force per unit mass felt in the transformed coordinates. This agrees with the approach of Ahmadi (1987), who investigated material frame-indifference for turbulence models using ensemble averages.

Now, the transformed momentum equation (3.54) becomes

$$\frac{\mathrm{D}\mathbf{u}^*}{\mathrm{D}t^*} = -\nabla^* p^* + \nu \nabla^{*2} \mathbf{u}^* + \mathbf{F}^*. \tag{3.57}$$

Checking that the mass conservation equation $\nabla \cdot \mathbf{u} = 0$ takes the same form in the new frame, we have shown that the Navier–Stokes equations are covariant, provided we define $\mathbf{F}^*$ to include the extra fictitious forces brought about by the change to a non-inertial frame.

Speziale (1985*b*) did not consider a body force acting on the fluid, so the fictitious forces introduced by the rotating frame meant that the momentum equation did not take the same form after transformation. However Ahmadi (1987) realised that the extra terms took the expected form for these fictitious forces, as we showed above. Since the NSEs take the same form in the transformed frame, the filtered equations derived in either frame will also take the same form. Thus, the filtered NSEs with a body force are frame invariant provided that the body force transforms in a way that takes care of the appearance of fictitious forces in a rotating frame.

Chapter 4

Dynamic Eddy Viscosity Models

4.1 The Eddy Viscosity Hypothesis

Richardson (1922) introduced the idea of an energy cascade, where energy enters the flow at large scales and is transferred locally in wavenumber space to smaller scales. Eventually, the energy is dissipated by viscous effects, which become important at sufficiently small length scales. As mentioned in Chapter 1, Kolmogorov (1941) proposed that in the inertial range, the energy flux in wavenumber space should be independent of the wavenumber k. It therefore makes sense for the subgrid tensor $\boldsymbol{\tau}$ to reproduce the effect of this constant energy flux, since $\boldsymbol{\tau}$ represents the interaction between the resolved scales and the subgrid scales.

Berselli *et al.* (2006) noted that Boussinesq proposed an Eddy Viscosity hypothesis in 1877, well before the idea of an energy cascade was introduced, by suggesting an analogy between Brownian motion and the interactions of the small eddies. We can apply this idea to LES by introducing a subgrid viscosity $\nu_{sgs} \geq 0$ to model the interactions of the subgrid-scale fluctuations with the resolved scales. Mathematically, we express this as

$$\boldsymbol{\tau}^d = 2\nu_{sgs}\langle \mathbf{s} \rangle, \tag{4.1}$$

where

$$s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{4.2}$$

is the rate-of-strain tensor for the fluid, the symmetric part of the velocity gradient, and

$$\tau_{ij}^d = \tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk}, \tag{4.3}$$

is the deviatoric (traceless) part of the subgrid-scale stress tensor. We choose to use this form in (4.1) so that the model remains consistent with incompressible flows, in which $\mathbf{s}$ is traceless:

$$s_{kk} = \nabla \cdot \mathbf{u} = 0. \tag{4.4}$$

Relating $\boldsymbol{\tau}$ to the rate-of-strain tensor $\mathbf{s}$ as in (4.1) is a good idea, since $\mathbf{s}$ satisfies all of the physical conditions that we discussed for $\boldsymbol{\tau}$ in Chapter 3. We also note that decomposing a general rank-2 tensor into its antisymmetric, trace, and symmetric-traceless parts is the most general decomposition that is irreducible under rotations. Thus, our definition of the symmetric tensor $\boldsymbol{\tau}$ in terms of its deviatoric part is justified, so long as our model for ν_{sgs} is also frame-indifferent.

We can add the trace of $\boldsymbol{\tau}$ to the filtered pressure term, so it is calculated explicitly from the filtered NSEs, and does not need prescribing. In practice, care must be taken here, since the calculated average pressure may take an inaccurate value when the generalized subgrid kinetic energy becomes large (i.e. τ_{kk} is large) (Sagaut, 2006). This provides further justification for imposing the realizability conditions discussed in section 3.3, which provide us with an upper bound for the turbulent kinetic energy.

Using the eddy viscosity hypothesis (4.1), the closure problem for the filtered NSEs is now reduced to finding an appropriate choice of the single scalar ν_{sgs} instead of trying to prescribe every component of $\boldsymbol{\tau}$. An overview of the development of this problem will now be discussed in the following sections.

4.2 The Smagorinsky Model

One of the simplest implementations of the eddy viscosity idea was first used for atmospheric flows by Smagorinsky (1963). This model is derived using two assumptions:

1. The dimensional analysis result

$$\nu_{sgs} \propto \Delta^{4/3}\mathcal{E}^{1/3}, \tag{4.5}$$

   where Δ is the characteristic cutoff length scale of the filter, and $\mathcal{E}$ is the turbulent dissipation density. In Chapter 1, we considered the volume integral of $\mathcal{E}$, which we referred to as ϵ, when describing the work of Kolmogorov (1941).

2. The turbulent dissipation density $\mathcal{E}$ is given by

$$\mathcal{E} = -\tau_{ij}\langle s_{ij}\rangle = -\tau^d_{ij}\langle s_{ij}\rangle, \tag{4.6}$$

   as obtained from equation (3.26) for the evolution of the generalized turbulent energy.

By substituting (4.6) into (4.5), and using the eddy viscosity assumption (4.1) we obtain

$$\nu^3_{sgs} \propto \Delta^4\tau^d_{ij}\langle s_{ij}\rangle, \tag{4.7a}$$
$$\nu^3_{sgs} \propto \Delta^4\nu_{sgs}\langle s_{ij}\rangle\langle s_{ij}\rangle. \tag{4.7b}$$

Rearranging this gives us the final model:

$$\nu_{sgs} = c_S\Delta^2\left(\langle s_{ij}\rangle\langle s_{ij}\rangle\right)^{1/2}, \tag{4.8}$$

where c_S is a constant, known as the Smagorinsky coefficient. Now, apart from the filter itself, this constant is the only parameter that needs to be prescribed in the model. Lilly (1967) compared the turbulent dissipation of this model to the theoretical dissipation using the ideas of Kolmogorov (1941) and concluded that, assuming the turbulence is homogeneous and isotropic, the correct value to use was ${c_S}^{1/2} = 0.17$. However, in practice the Smagorinsky coefficient has often been determined experimentally, and Lilly's value is typically too large (Berselli *et al.*, 2006). In fact, when c_S is adjusted to improve results, different optimum values are obtained for different flows. Hence, the Smagorinsky model is not suited to modelling flows which exhibit multiple behaviours, e.g. flows undergoing transition to turbulence.

4.3 Germano's Dynamic Model

To overcome some of these issues with the Smagorinsky model, Germano (1992) proposed a model in which the coefficient c_S is determined dynamically at each stage of the numerical simulation. This is achieved by introducing a second 'test' filter at a slightly larger scale, and comparing what happens at this level to the existing filtered equations using a tensor relation now known as the Germano identity.

4.3.1 The Germano Identity

To avoid confusion, we will now refer to the filter used previously as the G-level filter and denote the filtered velocity by $\langle \mathbf{u} \rangle$. We define the test filter to be the T-level filter denoted by a bar symbol. The convolution definition of a filter operation establishes that these filters commute ($TG = GT$), so we may also define the doubly-filtered velocity as

$$\overline{\langle \mathbf{u} \rangle} = \langle \overline{\mathbf{u}} \rangle. \tag{4.9}$$

Now we must recall the notation of section 3.2, where $\tau(u_i, u_j)$ was used instead of the subgrid stress tensor τ_{ij} so that further generalised central moments could be defined. This allows us to easily differentiate between the subgrid-scale stresses at different levels of filtering:

$$\tau_G(u_i, u_j) = \langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle, \tag{4.10a}$$

$$\tau_T(u_i, u_j) = \overline{u_i u_j} - \overline{u_i}\,\overline{u_j}, \tag{4.10b}$$

$$\tau_{GT}(u_i, u_j) = \overline{\langle u_i u_j \rangle} - \overline{\langle u_i \rangle}\,\overline{\langle u_j \rangle}. \tag{4.10c}$$

By some simple rearranging of (4.10c), we arrive at the key tensor relation identified by Germano (1992):

$$\tau_{GT}(u_i, u_j) = \overline{\langle u_i u_j \rangle} - \overline{\langle u_i \rangle}\,\overline{\langle u_j \rangle} + \overline{\langle u_i \rangle \langle u_j \rangle} - \overline{\langle u_i \rangle \langle u_j \rangle}, \tag{4.11a}$$

$$= \overline{\langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle} + \overline{\langle u_i \rangle \langle u_j \rangle} - \overline{\langle u_i \rangle}\,\overline{\langle u_j \rangle}, \tag{4.11b}$$

$$\text{which implies} \quad \tau_{GT}(u_i, u_j) = \overline{\tau_G(u_i, u_j)} + \tau_T(\langle u_i \rangle, \langle u_j \rangle). \tag{4.12}$$

The final term in (4.12) is expressed using only the filtered velocities. Germano (1992) gave a physical interpretation of identity (4.12) as "the turbulent stress at the GT-level is equal to the T-averaged value of the turbulent stress at the G-level plus the resolved turbulent stress $\tau_T(\langle u_i \rangle, \langle u_j \rangle)$ extracted from the resolved scale G."

4.3.2 Germano's Method

To see how identity (4.12) will help us turn the Smagorinsky model into a dynamic model, we try substituting the expression for $\tau_G(u_i, u_j)$ obtained from the Smagorinsky model into the Germano identity. The full expression for the stress tensor comes from combining the eddy viscosity assumption (4.1) with the derived eddy viscosity expression (4.8):

$$\tau_G^d(u_i, u_j) = -2c_S\Delta^2 \left(\langle s_{kl} \rangle \langle s_{kl} \rangle\right)^{1/2} \langle s_{ij} \rangle. \tag{4.13}$$

As before, the left side of this equation represents the deviatoric part of the subgrid-scale stress tensor:

$$\tau_G^d(u_i, u_j) = \tau_G(u_i, u_j) - \frac{1}{3}\delta_{ij}\tau_G(u_k, u_k). \tag{4.14}$$

Replacing the unresolved terms in the Germano identity (4.12) with the above expression gives

$$-2c_S\Delta^2\left(\overline{\langle s_{kl}\rangle}\,\overline{\langle s_{kl}\rangle}\right)^{1/2}\overline{\langle s_{ij}\rangle} = -2c_S\overline{\Delta}^2\,\overline{(\langle s_{kl}\rangle\langle s_{kl}\rangle)^{1/2}\langle s_{ij}\rangle} + \tau_T^d(\langle u_i\rangle,\langle u_j\rangle), \tag{4.15}$$

where $\overline{\Delta}$ is the characteristic length scale of the test filter. Meneveau & Katz (2000) pointed out that this step assumes that c_S is scale invariant, i.e. that c_S should take the same value at the test scale as at the resolved scale. Since they also noted that the most commonly used test scale is $\overline{\Delta} = 2\Delta$, this is a reasonable assumption to make.

Equation (4.15) in fact consists of 5 separate equations, since $\boldsymbol{\tau}^d$ is a traceless, symmetric 3×3 tensor. Hence, each of the 5 components of (4.15) would be satisfied by a (typically) different value of c_S. To obtain a single value for c_S, Germano proposed that we define the dissipation at the GT-level to be

$$\mathcal{E}_{GT} = -\tau_{GT}^d(u_i,u_j)\overline{\langle s_{ij}\rangle}, \tag{4.16}$$

motivated by our earlier assumption (4.6). Contracting equation (4.15) with $\overline{\langle s_{ij}\rangle}$ gives us a single equation for calculating the value of c_S at each grid point, which relates the dissipation at the different filter levels.

We now have a self-adapting model that will adjust its parameters to suit the flow regime. This means that the model behaves more realistically than the Smagorinsky model in important situations such as transitions between turbulent and laminar flow (Germano *et al.*, 1991). However, there are weaknesses in the method. For example, Ghosal *et al.* (1995) pointed out that in obtaining equation (4.15) we have taken c_S outside of the T-filter on the right as if it were a constant. This has no real justification now we are using a dynamic method to calculate c_S at each point on our grid, so more care should be taken.

The remaining sections in this chapter will outline further areas where Germano's model needs development. We will show how modifications to Germano's dynamic model have been made to retain its modelling advantages while improving the mathematical basis on which it is founded.

4.3.3 Lilly's Improvement

For notational convenience, from now on we will return to using τ_{ij} as the subgrid stress tensor, with T_{ij} denoting the GT-scale tensor previously defined as $\tau_{GT}(u_i,u_j)$. The Germano identity (4.12) can then be rewritten as

$$K_{ij} = T_{ij} - \tau_{ij}, \tag{4.17}$$

where $K_{ij} = \tau_T(\langle u_i\rangle,\langle u_j\rangle)$ is the resolved stress. In this concise notation, we can rewrite the particular relation (4.15) as

$$K_{ij}^d = c_S(\alpha_{ij} - \overline{\beta_{ij}}), \tag{4.18}$$

where

$$\alpha_{ij} = -2\Delta^2\left(\overline{\langle s_{kl}\rangle}\,\overline{\langle s_{kl}\rangle}\right)^{1/2}\overline{\langle s_{ij}\rangle}, \tag{4.19a}$$

$$\beta_{ij} = -2\overline{\Delta}^2\left(\langle s_{kl}\rangle\langle s_{kl}\rangle\right)^{1/2}\langle s_{ij}\rangle. \tag{4.19b}$$

Contracting with $\overline{\langle s_{ij} \rangle}$ gives the following expression for c_S:

$$c_S = \frac{K_{ij}\overline{\langle s_{ij} \rangle}}{(\alpha_{ij} - \overline{\beta_{ij}})\overline{\langle s_{ij} \rangle}}. \tag{4.20}$$

In an incompressible flow, s_{ij} is traceless, so there is no need to specify the deviatoric part of K_{ij}. However, when using (4.20) c_S can become indeterminate, with problems arising when the rate-of-strain tensor s_{ij} is small. Small values of s_{ij} mean that the flow is relatively smooth so the filter has less effect on the flow quantities. Hence, α_{ij} and $\overline{\beta_{ij}}$ will take similar values. As Germano *et al.* (1991) found, this can lead to the computation becoming unstable, so they averaged the numerator and denominator over planes parallel to the boundaries, assuming homogeneity of the flow in these directions. This approach cannot be used for inhomogeneous flows in complex domains.

Lilly (1992) proposed an alternative method to remove the redundancy in relation (4.18). Since a single value of c_S cannot typically satisfy all 5 independent components of the tensor relation, Lilly (1992) proposed taking a least squares approach to optimise the choice of c_S. First, we define the error tensor E_{ij} by

$$E_{ij} = K_{ij}^d - c_S(\alpha_{ij} - \overline{\beta_{ij}}). \tag{4.21}$$

In a least squares approach, we want to find the c_S that minimises the quantity $Q = E_{ij}E_{ij}$. Differentiating this quantity gives

$$\frac{\partial Q}{\partial c_S} = 2(\alpha_{ij} - \overline{\beta_{ij}}) \left(c_S(\alpha_{ij} - \overline{\beta_{ij}}) - K_{ij}^d \right), \tag{4.22}$$

and setting this derivative to zero to find an extremum produces a new expression for the Smagorinsky coefficient:

$$c_S = \frac{K_{ij}(\alpha_{ij} - \overline{\beta_{ij}})}{(\alpha_{ij} - \overline{\beta_{ij}})^2}. \tag{4.23}$$

Differentiating Q again confirms that this value does indeed minimise the square of the error:

$$\frac{\partial^2 Q}{\partial {c_S}^2} = 2(\alpha_{ij} - \overline{\beta_{ij}})^2 \geq 0. \tag{4.24}$$

The new c_S expression (4.23) has the advantage of only becoming indeterminate when all of the components of $\alpha_{ij} - \overline{\beta_{ij}}$ are zero.

The numerator of (4.23) can be either positive or negative locally. A negative value would indicate a negative eddy viscosity, which causes the opposite action to that suggested by the Boussinesq hypothesis: the kinetic energy would be transferred from the small scales to the large scales. This is known as backscatter and does occur in fluid flow due to the randomness inherent in turbulence. In fact, Piomelli *et al.* (1991) found from performing DNS for turbulent flow that the energy transfer between scales is large in both directions, and the eddy viscosity hypothesis of a mean diffusive effect is only valid due to a slight difference favouring the transfer to smaller scales. However, in regions near boundaries, the mean energy transfer was found to be reversed, which casts doubt on the validity of eddy viscosity models close to walls.

Hence, Lilly regarded the possibility of a negative subgrid viscosity as an advantage for the dynamic model, although negative values of c_S have since been found to cause numerical instabilities when the model is actually implemented (Meneveau & Katz, 2000). Intuitively, this makes sense as a negative subgrid viscosity would correspond analytically to a backward diffusion equation. This problem is well-known to be ill-posed, and can have solutions blowing up in infinitesimal time (Ockendon *et al.*, 1999).

4.4 A Constrained Variational Formulation

Ghosal *et al.* (1995) appreciated the advantage of the dynamic model in being self-calibrating for any flow situation, and formulated a new approach to overcome the deficiencies of the original Germano model. Some earlier papers (e.g. Zang *et al.*, 1993) attempted to adapt Germano's method for use in inhomogeneous flows by averaging over a small neighbourhood of grid points, rather than a symmetry plane, to smooth out variations in c_S, and sometimes 'clipped' negative values by setting them to zero.

This approach seemed rather "ad hoc" to Ghosal *et al.* (1995), who proposed a more mathematically consistent model for calculating the value of the Smagorinsky coefficient c_S. As noted before, we will start by correcting a rather brash assumption made in the derivation of Germano's method. When progressing from the Germano identity (4.17), substituting in the Smagorinsky closure model should have given us

$$K_{ij}^d = c_S \alpha_{ij} - \overline{c_S \beta_{ij}}, \tag{4.25}$$

where α_{ij} and β_{ij} are defined as before in (4.19a) and (4.19b). Since we are taking $c_S = c_S(\mathbf{x}, t)$, this coefficient remains inside the test filter operation, whereas before it was taken outside. Now we may redefine the error that Lilly (1992) proposed, but with our new consistent tensor relation:

$$E_{ij}(\mathbf{x}, t) = K_{ij}^d - c_S \alpha_{ij} + \overline{c_S \beta_{ij}}. \tag{4.26}$$

Ghosal *et al.* (1995) pointed out that minimising the square of the error locally, as Lilly (1992) suggested, is flawed. Changing c_S to minimise the value of $Q = E_{ij}E_{ij}$ at one location would alter the value of Q at adjacent points due to c_S being inside the filter in the last term of (4.26). Therefore, we should use the calculus of variations to minimise the spatial integral of Q as a functional of c_S at each time t:

$$\mathcal{F}[c_S](t) = \int_D E_{ij}(\mathbf{x}, t) E_{ij}(\mathbf{x}, t) \, \mathrm{d}\mathbf{x}. \tag{4.27}$$

In the following derivation we will neglect time dependence, since each minimisation is performed at a particular time t. Consider a small variation $c_S \to c_S + \delta c_S$. Under this variation, the functional $\mathcal{F}$ becomes

$$\mathcal{F}[c_S + \delta c_S] = \int_D (E_{ij} + \delta E_{ij})(E_{ij} + \delta E_{ij}) \, \mathrm{d}\mathbf{x}, \tag{4.28}$$

where $\delta E_{ij} = -\delta c_S \alpha_{ij} + \overline{\delta c_S \beta_{ij}}$. Expanding this out gives

$$\begin{aligned} \mathcal{F}[c_S + \delta c_S] &= \int_D E_{ij} E_{ij} \, \mathrm{d}\mathbf{x} + 2 \int_D E_{ij} \delta E_{ij} \, \mathrm{d}\mathbf{x} + O(\delta {E_{ij}}^2), && \text{(4.29a)} \\ &= \mathcal{F}[c_S] + \delta \mathcal{F}[c_S] + O(\delta {c_S}^2), && \text{(4.29b)} \end{aligned}$$

where $\delta\mathcal{F}$ is the first variation of the functional, as defined by

$$\delta \mathcal{F}[c_S] = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{F}[c_S + \epsilon \delta c_S]. \tag{4.30}$$

To find the Euler–Lagrange equation that can be used to calculate the minimising function c_S, we set the first variation $\delta\mathcal{F}$ to zero. The $O(\delta {E_{ij}}^2)$ term arising from (4.28)

is the integral of a positive quantity, so this ensures that we get a minimum for $\mathcal{F}$, not another type of stationary value. Using the definition of δE_{ij} from above, $\delta\mathcal{F}$ can be written as

$$\begin{aligned}\delta\mathcal{F} = &-2\int_D \alpha_{ij}(\mathbf{x})E_{ij}(\mathbf{x})\delta c_S(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &+2\int_D E_{ij}(\mathbf{x})\int_D G_T(\mathbf{x}-\mathbf{y})\beta_{ij}(\mathbf{y})\delta c_S(\mathbf{y})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{x},\end{aligned} \tag{4.31}$$

where G_T is the convolution kernel corresponding to the test filter. Swapping the independent variables in the second integral, combining the terms, and setting $\delta\mathcal{F}$ to zero gives

$$\int_D \left(-\alpha_{ij}(\mathbf{x})E_{ij}(\mathbf{x}) + \beta_{ij}(\mathbf{x})\int_D G_T(\mathbf{y}-\mathbf{x})E_{ij}(\mathbf{y})\,\mathrm{d}\mathbf{y}\right)\delta c_S(\mathbf{x})\,\mathrm{d}\mathbf{x} = 0. \tag{4.32}$$

This integral equation must hold for all small variations δc_S, which implies the Euler–Lagrange equation

$$-\alpha_{ij}(\mathbf{x})E_{ij}(\mathbf{x}) + \beta_{ij}(\mathbf{x})\int_D G_T(\mathbf{y}-\mathbf{x})E_{ij}(\mathbf{y})\,\mathrm{d}\mathbf{y} = 0. \tag{4.33}$$

We can now use the earlier definition of E_{ij} in (4.26) to express this integral equation in terms of c_S

$$\begin{aligned}&-\alpha_{ij}K_{ij}^d + \beta_{ij}\int_D K_{ij}^d(\mathbf{y})G_T(\mathbf{y}-\mathbf{x})\,\mathrm{d}\mathbf{y} \\ &\quad = \alpha_{ij}[-\alpha_{ij}c_S + \overline{\beta_{ij}c_S}] - \beta_{ij}\int_D G(\mathbf{y}-\mathbf{x})[-\alpha_{ij}c_S + \overline{\beta_{ij}c_S}](\mathbf{y})\,\mathrm{d}\mathbf{y}.\end{aligned} \tag{4.34}$$

Ghosal *et al.* (1995) spotted that dividing both sides by $\alpha_{kl}\alpha_{kl}$ gives a Fredholm integral equation of the second kind:

$$f(\mathbf{x}) = c_S(\mathbf{x}) - \int_D \mathcal{K}(\mathbf{x},\mathbf{y})c_S(\mathbf{y})\,\mathrm{d}\mathbf{y}, \tag{4.35}$$

where

$$f(\mathbf{x}) = \frac{1}{\alpha_{kl}(\mathbf{x})\alpha_{kl}(\mathbf{x})}\left[\alpha_{ij}(\mathbf{x})K_{ij}(\mathbf{x}) - \beta_{ij}(\mathbf{x})\int_D K_{ij}(\mathbf{y})G_T(\mathbf{y}-\mathbf{x})\,\mathrm{d}\mathbf{y}\right], \tag{4.36}$$

and

$$\begin{aligned}\mathcal{K}(\mathbf{x},\mathbf{y}) = \frac{1}{\alpha_{kl}(\mathbf{x})\alpha_{kl}(\mathbf{x})}\Big[&\alpha_{ij}(\mathbf{x})\beta_{ij}(\mathbf{y})G_T(\mathbf{x}-\mathbf{y}) + \alpha_{ij}(\mathbf{y})\beta_{ij}(\mathbf{x})G_T(\mathbf{y}-\mathbf{x}) \\ &- \beta_{ij}(\mathbf{x})\beta_{ij}(\mathbf{y})\int_D G(\mathbf{z}-\mathbf{x})G(\mathbf{z}-\mathbf{y})\,\mathrm{d}\mathbf{z}\Big].\end{aligned} \tag{4.37}$$

If we define the right hand side of this equation to be the integral operator $\mathfrak{L}$, then as long as there are no eigenfunctions c_0 which satisfy $\mathfrak{L}c_0 = 0$, the above equation will always have a unique solution (Collins, 2006).

This formulation resolves the issue of removing c_S from the filter, but does not tackle the instability problem of the dynamic model. Ghosal *et al.* (1995) proposed two methods

for overcoming this, the first of which requires that c_S be non-negative. To achieve this, they introduced a new variable γ and wrote $c_S = \gamma^2$. Reformulating the integral (4.32) with $\delta c_S(\mathbf{x}) = 2\gamma(\mathbf{x})\delta\gamma(\mathbf{x})$ and $E_{ij} = K_{ij}^d - \gamma^2\alpha_{ij} + \overline{\gamma^2\beta_{ij}}$,

$$\int_D \left(-\alpha_{ij}(\mathbf{x})E_{ij}(\mathbf{x}) + \beta_{ij}(\mathbf{x}) \int_D G_T(\mathbf{y}-\mathbf{x})E_{ij}(\mathbf{y})\,\mathrm{d}\mathbf{y} \right) \gamma(\mathbf{x})\delta\gamma(\mathbf{x})\,\mathrm{d}\mathbf{x} = 0. \tag{4.38}$$

This gives us a new Euler–Lagrange equation

$$\left(-\alpha_{ij}(\mathbf{x})E_{ij}(\mathbf{x}) + \beta_{ij}(\mathbf{x}) \int_D G_T(\mathbf{y}-\mathbf{x})E_{ij}(\mathbf{y})\,\mathrm{d}\mathbf{y} \right) \gamma(\mathbf{x}) = 0. \tag{4.39}$$

However, we now always have $\gamma(\mathbf{x}) = 0$ as a solution, in addition to $\gamma(\mathbf{x}) = c_S(\mathbf{x})^{1/2}$ where $c_S(\mathbf{x})$ is a positive solution to (4.35). To avoid this trivial second solution, while still enforcing $c_S(\mathbf{x}) \geq 0$, we can use the iterative procedure

$$c_S^{(n+1)}(\mathbf{x}) = \begin{cases} f(\mathbf{x}) + \int_D \mathcal{K}(\mathbf{x},\mathbf{y}) c_S^{(n)}(\mathbf{y})\,\mathrm{d}\mathbf{y}, & \text{if this} \geq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.40}$$

Although we have not established that this iteration always converges, Ghosal *et al.* (1995) found no issues from lack of convergence in their numerical simulations. We now have a dynamic model which remains stable in flows without any symmetry (inhomogeneous flows). This is a key development over the previous models by Germano *et al.* (1991) and Lilly (1992), which would become unstable in these regimes.

The second formulation proposed by Ghosal *et al.* (1995) involves modelling the backscatter process to allow negative values of c_S without causing instability in its calculation. This model is rather elaborate, and we will not cover the finer details here. The key idea is that the energy spectrum $E(k)$, introduced in Chapter 1, must be realizable, in the sense that (Sagaut, 2006)

$$E(k) \geq 0 \quad \text{for all } k, \tag{4.41}$$

since (1.4) defines $E(k)$ as the integral of a non-negative quantity. The subgrid-scale kinetic energy E_T (recall (3.25)) is added as a variable in the system, along with a transport equation which ensures (4.41). Now, when c_S becomes negative, E_T decreases. When the energy contained at the subgrid level reaches zero the subgrid stresses τ_{ij}, and hence c_S, must also be zero. This means that a negative value of c_S does not lead to computational instability.

Carati *et al.* (1995) showed that the dynamic Ghosal *et al.* (1995) model which includes an equation for E_T produces more accurate results for numerical simulations of isotropic turbulence than the original dynamic models of Germano *et al.* (1991) and Lilly (1992). In fact, all of the developments throughout this chapter have improved the accuracy of simulations produced by eddy viscosity models, reassuring us that improving the mathematical underpinnings of a model should also improve the results we obtain when using it.

Chapter 5

Regularized Models

In this chapter, we describe an alternative approach for finding a closure model for $\boldsymbol{\tau}$. Unlike in Chapter 4, this approach does not produce models which satisfy the constraints derived in Chapter 3, and so requires modification.

5.1 Leray Regularization

5.1.1 Leray's 1934 Paper

Although the Navier–Stokes equations have been ubiquitous in the field of fluid mechanics for some time, mathematical understanding of their solutions is limited. In fact, one of the Clay Mathematics Institute's (unsolved) Millenium Prize Problems is to establish existence and regularity of solutions to the Navier–Stokes equations in $\mathbb{R}^3$ (Ladyzhenskaya, 2003; Fefferman, 2000).

Much of the work in trying to prove existence and regularity of solutions of the NSEs can trace its roots back to a ground-breaking paper by Leray (1934), which introduced the idea of weak solutions of the Navier–Stokes equations (referred to as "turbulent solutions" in that paper). Leray (1934) proposed a regularized form of the Navier–Stokes equations that smoothed out the advective term, resulting in the following equations:

$$\nabla \cdot \mathbf{u} = 0, \tag{5.1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}, \tag{5.2}$$

where $\overline{\mathbf{u}}$ is defined by

$$\overline{\mathbf{u}}(\mathbf{x}, t) = [\phi_\epsilon * \mathbf{u}](\mathbf{x}, t) = \int_{\mathbb{R}^3} \phi_\epsilon(\mathbf{x} - \boldsymbol{\xi}) \mathbf{u}(\boldsymbol{\xi}, t) d\boldsymbol{\xi}, \tag{5.3}$$

and $\phi_\epsilon \in C_0^\infty(\mathbb{R}^3)$ is a smooth 'mollifying' function which integrates to 1 over $\mathbb{R}^3$, and is assumed to have compact support within a ball of radius ϵ (i.e. $\text{supp}(\phi_\epsilon) \subset B(0, \epsilon)$).

Leray proved that, for periodic boundary conditions and smooth initial conditions, equations (5.1) and (5.2) have a unique solution, and that this solution remains bounded for all time.

5.1.2 Interpretation as a LES Model

From an analytical perspective, the result is most interesting in the limit when $\epsilon \to 0$, since it provides insight into weak solutions of the NSEs. However, in the context of this dissertation, we can use this uniqueness result as justification for a different approach to LES.

Leray's definition of a smoothed velocity $\overline{\mathbf{u}}$ closely resembles that of the filtered velocity introduced in LES. Following the approach of Geurts & Holm (2003), if we perform this smoothing operation to the whole of Leray's momentum equation (5.2), and denote the average by the same filtering notation as before, a familiar equation arises:

$$\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{u} \rangle \langle \mathbf{u} \rangle) = -\nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{u} \rangle - \nabla \cdot \mathbf{m}, \tag{5.4}$$

where the tensor $\mathbf{m}$ is now defined as

$$m_{ij} = \langle \langle u_i \rangle u_j \rangle - \langle u_i \rangle \langle u_j \rangle. \tag{5.5}$$

If we choose a filtering operation with a known inverse operator $\mathcal{L}$, such as a differential filter as introduced in section 2.2.1, we can express the Leray stress tensor $\mathbf{m}$ in terms of the filtered velocity components:

$$m_{ij} = \langle \langle u_i \rangle \mathcal{L}(\langle u_j \rangle) \rangle - \langle u_i \rangle \langle u_j \rangle. \tag{5.6}$$

This tensor is asymmetric, so very little of what was discussed in chapter 3 can be applied directly to the Leray stress tensor. However, compared to applying this idea to the previous subgrid-scale stress tensor, so that

$$\tau_{ij} = \langle \mathcal{L}(\langle u_i \rangle) \mathcal{L}(\langle u_j \rangle) \rangle - \langle u_i \rangle \langle u_j \rangle, \tag{5.7}$$

the Leray model produces more regular numerical solutions. According to Geurts & Holm (2003), when using the modified Helmholtz filter from section 2.2.1, model (5.7) "does not provide sufficient smoothing and leads to unstable LES on coarse grids". Since analytic solutions to Leray's regularized equations are more well-behaved, regarding smoothness and boundedness, than solutions to the NSEs, it makes sense that the implementation of Leray's equations as a numerical model improves simulation results.

Using the modified Helmholtz filter

$$\mathcal{L}(\langle \mathbf{u} \rangle) = \langle \mathbf{u} \rangle - \alpha^2 \nabla^2 \langle \mathbf{u} \rangle, \tag{5.8}$$

the Leray stress tensor becomes

$$m_{ij} = \alpha^2 u_i \nabla^2 \langle u_j \rangle. \tag{5.9}$$

We will use α as the cutoff length scale for the filter in this chapter, rather than Δ, to avoid confusion with differential operators. In this case, we can see that the tensor is formally small, with $|\mathbf{m}| \sim \alpha^2$. Since the Leray tensor is not of the same form as the subgrid-scale stress tensor, we should take a different approach when considering how the regularized equations transform under a generic change of reference frame. Guermond *et al.* (2003) asserted that "a necessary and sufficient condition for frame indifference is that the momentum equation [can] be expressed in the form

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (q\mathbf{I} + \mathbf{T}), \tag{5.10}$$

where q is a scalar function, $\mathbf{I}$ the identity tensor and $\mathbf{T}$ a frame-indifferent tensor." This is a stronger condition than the one we derived for $\boldsymbol{\tau}$ and the filtered equations in chapter 3, when we showed that $\nabla \cdot \boldsymbol{\tau}$ should be frame-indifferent, even if $\boldsymbol{\tau}$ itself is not. We will thus require the momentum equation to take the form (5.10), with $\nabla \cdot \mathbf{T}$ being frame-indifferent.

Using this result, we can investigate Leray's regularized equations by writing the momentum equation in the form

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} - \left(\langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u} \right). \tag{5.11}$$

Comparing the above equation with condition (5.10), we can see that the regularized equations can only be frame-indifferent if $\langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u}$ can be expressed as the frame-indifferent divergence of a tensor. Hence, this expression must be also exhibit frame indifference itself. However, from Chapter 3 we know that $\mathbf{u}' = \mathbf{u} - \langle \mathbf{u} \rangle$ is indifferent under a general Euclidean transformation, but the tensor $\nabla \mathbf{u}$ is not:

$$\mathbf{x}^* = Q(t)\mathbf{x} + \mathbf{b}(t), \qquad QQ^T = I, \tag{5.12a}$$

$$\mathbf{u} = Q^T(\mathbf{u}^* - \dot{Q}Q^T(\mathbf{x}^* - \mathbf{b}) - \dot{\mathbf{b}}), \tag{5.12b}$$

so

$$(\nabla \mathbf{u})_{ij} = \frac{\partial u_j}{\partial x_i} = Q_{lj} \left(\frac{\partial {u_l}^*}{\partial {x_k}^*} + {\Omega^\wedge}_{lm} \frac{\partial {x_m}^*}{\partial {x_k}^*} \right) Q_{ki}. \tag{5.12c}$$

In vector notation, this becomes

$$\nabla \mathbf{u} = Q^T \nabla^* \mathbf{u}^* Q + \boldsymbol{\Omega}^\wedge, \qquad \text{where} \quad \boldsymbol{\Omega}^\wedge = Q\dot{Q}^T = -\dot{Q}Q^T. \tag{5.13}$$

Note that we are now using $\boldsymbol{\Omega}^\wedge$ to represent the antisymmetric tensor, rather than expressing multiplication by this tensor with a cross product as in chapter 3. Since $\boldsymbol{\Omega}^\wedge$ is antisymmetric, we can also define it in the sense of a vorticity tensor, using (5.13):

$$\boldsymbol{\Omega}^\wedge = \frac{1}{2} \left(\nabla \mathbf{u} - (\nabla \mathbf{u})^T \right). \tag{5.14}$$

Leray's regularized equations are therefore not frame indifferent, so using them as the basis for a model for the Navier–Stokes equations may cause problems when simulating a rotating fluid. We should now check the filtered equations themselves to ensure that our suspicions about this model are correct. To do this, we must introduce the Jaumann derivative $\breve{\mathbf{s}}$, the corotational form of the material derivative of the rate-of-strain tensor, i.e.

$$\breve{\mathbf{s}} = Q^T \frac{\mathrm{D}\mathbf{s}^*}{\mathrm{D}t} Q, \qquad \text{where} \quad \mathbf{s} = \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right). \tag{5.15}$$

This quantity was originally proposed for use in a rheological context, and has been useful for developing rotationally invariant models of viscoelastic fluids (see Bird *et al.*, 1977). We can also derive an alternative form for the Jaumann derivative by performing the chain rule on $\mathrm{D}\mathbf{s}^*/\mathrm{D}t$:

$$\frac{\mathrm{D}\mathbf{s}^*}{\mathrm{D}t} = \dot{Q}\mathbf{s}Q^T + Q\frac{\mathrm{D}\mathbf{s}}{\mathrm{D}t}Q^T + Q\mathbf{s}\dot{Q}^T, \tag{5.16}$$

which, after pre-multiplication by Q^T and post-multiplication by Q, gives

$$\breve{\mathbf{s}} = \frac{\partial \mathbf{s}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{s} + \mathbf{s} \cdot \boldsymbol{\Omega}^\wedge - \boldsymbol{\Omega}^\wedge \cdot \mathbf{s}. \tag{5.17}$$

Guermond *et al.* (2003) stated that the $\mathbf{T}$ that appears in the momentum equation (5.10) is frame-indifferent if and only if it depends only on the rate-of-strain tensor $\mathbf{s}$ and its Jaumann derivative $\check{\mathbf{s}}$. To take advantage of this condition, we can obtain the Helmholtz-filtered equations in an alternative way, and apply the inverse operator $\mathcal{L}$ to the Leray momentum equation (5.11) directly:

$$\begin{aligned}\frac{\partial}{\partial t}\left((1-\alpha^2\nabla^2)\langle\mathbf{u}\rangle\right) + \langle\mathbf{u}\rangle\cdot\nabla\left((1-\alpha^2\nabla^2)\langle\mathbf{u}\rangle\right) \\ = -\nabla\langle p\rangle + \nu\nabla^2\left((1-\alpha^2\nabla^2)\langle\mathbf{u}\rangle\right).\end{aligned} \tag{5.18}$$

This rearranges into

$$\begin{aligned}\frac{\partial\langle\mathbf{u}\rangle}{\partial t} + \langle\mathbf{u}\rangle\cdot\nabla\langle\mathbf{u}\rangle = -\nabla\langle p\rangle + \nu\nabla^2\langle\mathbf{u}\rangle \\ + \alpha^2\left[\frac{\partial}{\partial t}\left(\nabla^2\langle\mathbf{u}\rangle\right) + \langle\mathbf{u}\rangle\cdot\nabla(\nabla^2\langle\mathbf{u}\rangle) - \nu\nabla^4\langle\mathbf{u}\rangle\right].\end{aligned} \tag{5.19}$$

To apply the frame-indifference condition stated above to the filtered equation, we need to consider the Jaumann derivative of the filtered variables. Since the filter operation commutes with derivatives, the divergence of $\langle\check{\mathbf{s}}\rangle$ is given by (Guermond *et al.*, 2003)

$$2\nabla\cdot\langle\check{\mathbf{s}}\rangle = \frac{\partial}{\partial t}(\nabla\cdot\langle\mathbf{s}\rangle) + \langle\mathbf{u}\rangle\cdot\nabla(\nabla^2\langle\mathbf{u}\rangle) + \nabla(\langle\mathbf{s}\rangle:\langle\mathbf{s}\rangle) + (\nabla\langle\mathbf{u}\rangle)^T\cdot\nabla^2\langle\mathbf{u}\rangle, \tag{5.20}$$

where

$$\langle\mathbf{s}\rangle = \frac{1}{2}(\nabla\langle\mathbf{u}\rangle + (\nabla\langle\mathbf{u}\rangle)^T), \qquad \langle\mathbf{s}\rangle:\langle\mathbf{s}\rangle = \langle s_{ij}\rangle\langle s_{ij}\rangle, \tag{5.21}$$

and

$$\left((\nabla\langle\mathbf{u}\rangle)^T\cdot\nabla^2\langle\mathbf{u}\rangle\right)_i = \frac{\partial\langle u_j\rangle}{\partial x_i}\nabla^2\langle u_j\rangle. \tag{5.22}$$

Noting that $\nabla\cdot\langle\mathbf{s}\rangle = \nabla^2\langle\mathbf{u}\rangle$, we spot that the first two terms of this divergence agree with terms in the filtered equation (5.19). Thus, we can write

$$\begin{aligned}\frac{\partial\langle\mathbf{u}\rangle}{\partial t} + \langle\mathbf{u}\rangle\cdot\nabla\langle\mathbf{u}\rangle = \nabla\cdot\left((-\langle p\rangle + \alpha^2\langle\mathbf{s}\rangle:\langle\mathbf{s}\rangle)\mathbf{I} + 2\nu(1-\alpha^2\nabla^2)\langle\mathbf{s}\rangle + 2\alpha^2\langle\check{\mathbf{s}}\rangle\right) \\ - \alpha^2(\nabla\langle\mathbf{u}\rangle)^T\cdot\nabla^2\langle\mathbf{u}\rangle.\end{aligned} \tag{5.23}$$

Comparing this with frame-indifference condition (5.10) from Guermond *et al.* (2003), we can see that an extra term has appeared, namely $-\alpha^2(\nabla\langle\mathbf{u}\rangle)^T\cdot\nabla^2\langle\mathbf{u}\rangle$. Previous results (see (5.13) and (3.53b)) establish that this extra term is not frame-indifferent, so the direct implementation of Leray's regularization as a model is not necessarily applicable for rotating fluids. However, it is worth noting that this term is proportional to α^2, so the error is often relatively small.

5.2 Navier–Stokes–α Model

To go about formulating a frame-indifferent adaptation of Leray's regularized equations we could just subtract the term that caused a problem in the last section from the equations. However, we gain more mathematical insight by first writing the Navier–Stokes momentum equation in an alternative form that is often used for rotational flows:

$$\frac{\partial \mathbf{u}}{\partial t} + (\nabla \wedge \mathbf{u}) \wedge \mathbf{u} = -\nabla \left(p + \frac{1}{2}|\mathbf{u}|^2 \right) + \nu \nabla^2 \mathbf{u}. \tag{5.24}$$

Using the same idea that Leray (1934) used to smooth equation (5.2), we can put the average velocity in the vorticity wedge term to obtain

$$\frac{\partial \mathbf{u}}{\partial t} + (\nabla \wedge \mathbf{u}) \wedge \langle \mathbf{u} \rangle = -\nabla \left(p + \frac{1}{2}|\mathbf{u}|^2 \right) + \nu \nabla^2 \mathbf{u}. \tag{5.25}$$

The following tensor calculus identities will help us manipulate this new equation:

$$(\nabla \wedge \mathbf{u}) \wedge \langle \mathbf{u} \rangle = \langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} - (\nabla \mathbf{u})^T \cdot \langle \mathbf{u} \rangle, \tag{5.26a}$$

$$\nabla(\mathbf{u} \cdot \langle \mathbf{u} \rangle) = (\nabla \mathbf{u})^T \cdot \langle \mathbf{u} \rangle + (\nabla \langle \mathbf{u} \rangle)^T \cdot \mathbf{u}. \tag{5.26b}$$

The vorticity-smoothed momentum equation (5.25) now becomes

$$\frac{\partial \mathbf{u}}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} + (\nabla \langle \mathbf{u} \rangle)^T \cdot \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u}, \tag{5.27}$$

where $P = p + \frac{1}{2}|\mathbf{u}|^2 - \mathbf{u} \cdot \langle \mathbf{u} \rangle$ is the modified pressure.

Before we try to relate these equations to the usual form of LES models, it is worth noting that we can prove a very interesting result for solutions to the above equation. Firstly, define the circulation around a closed material curve $C(t)$ being convected by the actual flow velocity $\mathbf{u}$ as

$$\Gamma = \int_{C(t)} \mathbf{u} \cdot \mathrm{d}\mathbf{x}. \tag{5.28}$$

Now consider the circulation around a closed curve $\hat{C}(t)$ which is convected by the filtered velocity $\langle \mathbf{u} \rangle$ instead. This can be expressed in terms of Lagrangian variables $\mathbf{X}$, that move with the filtered flow velocity over time, as

$$\hat{\Gamma} = \int_{\hat{C}(t)} \mathbf{u} \cdot \mathrm{d}\mathbf{x} = \int_{\hat{C}(0)} u_i \frac{\partial x_i}{\partial X_j} \, \mathrm{d}X_j. \tag{5.29}$$

The velocity inside the integral is still the actual velocity of the flow, while the closed curve $\hat{C}(t)$ is convected with the filtered velocity. Differentiating the circulation $\hat{\Gamma}$ with respect to time gives

$$\frac{\mathrm{d}\hat{\Gamma}}{\mathrm{d}t} = \int_{\hat{C}(0)} \frac{\mathrm{D}}{\mathrm{D}t} \left(u_i \frac{\partial x_i}{\partial X_j} \right) \mathrm{d}X_j, \tag{5.30}$$

where $\mathrm{D}/\mathrm{D}t$ is the material derivative following the *filtered* Langrangian variables, i.e.

$$\frac{\mathrm{D}}{\mathrm{D}t} = \left(\frac{\partial}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \right), \qquad \frac{\mathrm{D}\mathbf{x}}{\mathrm{D}t} = \langle \mathbf{u} \rangle. \tag{5.31}$$

We now use the product rule and apply the above definition:

$$\frac{\mathrm{d}\hat{\Gamma}}{\mathrm{d}t} = \int_{\hat{C}(0)} \left(\frac{\mathrm{D}u_i}{\mathrm{D}t} \frac{\partial x_i}{\partial X_j} + u_i \frac{\partial \langle u_i \rangle}{\partial X_j} \right) \mathrm{d}X_j, \tag{5.32a}$$

$$= \int_{\hat{C}(t)} \frac{\mathrm{D}u_i}{\mathrm{D}t} \, \mathrm{d}x_i + \int_{\hat{C}(t)} u_i \frac{\partial \langle u_i \rangle}{\partial x_j} \, \mathrm{d}x_j, \tag{5.32b}$$

$$= \int_{\hat{C}(t)} \left(\frac{\partial \mathbf{u}}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} + (\nabla \mathbf{u})^T \cdot \mathbf{u} \right) \cdot \mathrm{d}\mathbf{x}. \tag{5.32c}$$

Now we can use the smoothed momentum equation (5.27) to derive the following result:

$$\frac{\mathrm{d}\hat{\Gamma}}{\mathrm{d}t} = \int_{\hat{C}(t)} \nu \nabla^2 \mathbf{u} \cdot \mathrm{d}\mathbf{x}. \tag{5.33}$$

The above equation is essentially Kelvin's circulation theorem (as in Acheson, 1990) but with the curve $\hat{C}$ being convected with the filtered velocity $\langle \mathbf{u} \rangle$. This gives further physical justification for smoothing the momentum equation as we did in (5.25), and is in fact the result from which this approach, known as the Navier–Stokes-α model, was originally developed (see Foias *et al.*, 2001). Marsden & Shkoller (2002) refer to this technique as Lagrangian Averaged Navier–Stokes (LANS), since the idea of following the average fluid velocity used above is the key difference in thinking between regular LES models and this approach.

With this physical interpretation established, let us return to the vorticity-smoothed equation (5.27). Comparing this with the standard form of Leray's momentum equation, it appears that the only difference has arisen in the term $(\nabla \langle \mathbf{u} \rangle)^T \cdot \mathbf{u}$ and the modified pressure P. To investigate how these terms are expressed in the filtered equations, we apply the Helmholtz inverse operator to the velocities in each quantity:

$$(\nabla \langle \mathbf{u} \rangle)^T \cdot \mathbf{u} = (\nabla \langle \mathbf{u} \rangle)^T \cdot (\langle \mathbf{u} \rangle - \alpha^2 \nabla^2 \langle \mathbf{u} \rangle), \tag{5.34a}$$

$$= (\nabla \langle \mathbf{u} \rangle)^T \cdot \langle \mathbf{u} \rangle - \alpha^2 (\nabla \langle \mathbf{u} \rangle)^T \cdot \nabla^2 \langle \mathbf{u} \rangle, \tag{5.34b}$$

$$= \nabla \left(\frac{1}{2} |\langle \mathbf{u} \rangle|^2 \right) - \alpha^2 (\nabla \langle \mathbf{u} \rangle)^T \cdot \nabla^2 \langle \mathbf{u} \rangle. \tag{5.34c}$$

In the final line above we have made use of a particular case of the tensor calculus identity in (5.26b) when $\mathbf{u} = \langle \mathbf{u} \rangle$.

$$P = p + \frac{1}{2} |\mathbf{u}|^2 - \mathbf{u} \cdot \langle \mathbf{u} \rangle, \tag{5.35a}$$

$$= p + \frac{1}{2} (|\langle \mathbf{u} \rangle|^2 - 2\alpha^2 \langle \mathbf{u} \rangle \cdot \nabla^2 \langle \mathbf{u} \rangle + \alpha^4 |\nabla^2 \langle \mathbf{u} \rangle|^2) - |\langle \mathbf{u} \rangle|^2 + \alpha^2 \langle \mathbf{u} \rangle \cdot \nabla^2 \langle \mathbf{u} \rangle, \tag{5.35b}$$

$$= p - \frac{1}{2} (|\langle \mathbf{u} \rangle|^2 + \alpha^4 |\nabla^2 \langle \mathbf{u} \rangle|^2). \tag{5.35c}$$

Substituting expressions (5.34c) and (5.35c) into the vorticity-smoothed equation (5.27) without performing any further filtering or inversion operations gives us

$$\frac{\partial \mathbf{u}}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \mathbf{u} - \alpha^2 (\nabla \langle \mathbf{u} \rangle)^T \cdot \nabla^2 \langle \mathbf{u} \rangle = -\nabla \hat{p} + \nu \nabla^2 \mathbf{u}, \tag{5.36}$$

where $\hat{p} = p + \frac{1}{2} \alpha^4 |\nabla^2 \langle \mathbf{u} \rangle|^2$. Comparing this with the Leray implementation model, we now satisfy the frame-indifference condition from Guermond *et al.* (2003) since we have

subtracted the term which caused issues before, and have only added an extra gradient term. Thus, we have the form

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (q\mathbf{I} + \mathbf{T}), \tag{5.37}$$

where

$$q = -\langle p \rangle + \alpha^2 \mathbf{s} : \mathbf{s} - \frac{1}{2}\alpha^4 |\nabla^2 \langle \mathbf{u} \rangle|^2, \tag{5.38}$$

$$\mathbf{T} = 2\nu(1 - \alpha^2 \nabla^2)\mathbf{s} + 2\nabla^2 \check{\mathbf{s}}. \tag{5.39}$$

Hence, as Sagaut (2006) stated, we have found that the Navier–Stokes-α method arises as a frame-indifferent perturbation of order α^2 of the original Leray model. Its mathematical underpinnings are further justified by the form of Kelvin's theorem (5.33) that it satisfies. Understandably, this means the NS-α model produces results with more "realistic variability" than the Leray model. Geurts (2014) showed that the solutions provided by the NS-α model matched DNS results relatively closely, whereas the Leray model over-smoothed some of the turbulent flow behaviour. However, the Leray model showed itself to be more robust at high Reynolds numbers and produced better results than Germano's dynamic method discussed in section 4.3. Further research should widen the application of these regularization models, which are already showing much promise compared to the most commonly used LES models.

Chapter 6

Conclusion

Over the course of this dissertation, we have investigated the Large Eddy Simulation approach for modelling turbulent fluid flows. We started by outlining the theory of Kolmogorov (1941) which kick-started research on turbulent flow, before introducing scale separation and flow averaging using a filter in Chapter 2. We then highlighted some examples of spatial averages used in LES, including the idea of averaging using an invertible differential filter. We also derived the filtered Navier–Stokes equations, which contain the unresolved tensor $\boldsymbol{\tau}$ to account for the effect of the small scale fluctuations.

We need a closure model for $\boldsymbol{\tau}$ to evolve the filtered velocity, so in Chapter 3 we investigated which physical constraints should be imposed either on $\boldsymbol{\tau}$ or on the filter. We showed that the filter kernel should be spherically symmetric, and that $\nabla \cdot \boldsymbol{\tau}$ must be invariant under an arbitrary change of frame. We also introduced the idea of generalized turbulent energy, and showed that it is bounded if we use a positive filter.

To satisfy these conditions, we introduced an eddy viscosity model for $\boldsymbol{\tau}$, and derived the simple Smagorinsky (1963) implementation of this idea in Chapter 4. We explored the work of Germano (1992) to formulate a dynamic version of this implementation which adapts the eddy viscosity to the flow regime during a simulation. We highlighted the improvement made to this model by Lilly (1992), and derived a variational formulation proposed by Ghosal *et al.* (1995) based on the dynamic model that properly treats the Smagorinsky coefficient c_S as a function of space and time.

In Chapter 5, we introduced the notion of regularization of the Navier–Stokes equations proposed by Leray (1934) and highlighted the importance of this paper for the analysis of the NSEs. We then applied Leray's idea to LES using the modified Helmholtz filter, and showed that a direct implementation of regularization does not satisfy our frame-indifference condition. To resolve this problem, we formulated the Navier–Stokes-α model (Foias *et al.*, 2001) as a frame-indifferent perturbation of the original regularization.

Through development of the underlying mathematics of LES models, progress has been made in producing more accurate numerical simulations (see Carati *et al.*, 1995; Geurts, 2014). This gives us confidence that further research into the mathematical theory of LES will produce ever more reliable simulations in the future.

Large Eddy Simulation is a vast topic, and this dissertation has only focused on a small part of the modelling process. Many models have been proposed for LES which we have not discussed, for example using stochastic techniques (Sagaut, 2006). We have also mentioned very little about modelling turbulent flow near a boundary, which is key to many applications in engineering. The mathematical theory for LES is limited in many of these areas, where there is much scope for further research.

Appendix A

Central Moments Derivations

In section 3.2, we explored the idea of averaging invariance by introducing generalised central moments. We produced a number of equations involving these generalised moments, which are derived here in full.

Using notation from section 3.2, the Navier–Stokes momentum equation is

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_k}\left(u_i u_k\right) = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_k \partial x_k} + F_i. \tag{A.1}$$

We first multiply (A.1) by u_j:

$$u_j \frac{\partial u_i}{\partial t} + u_j \frac{\partial}{\partial x_k}\left(u_i u_k\right) = -u_j \frac{\partial p}{\partial x_i} + \nu u_j \frac{\partial^2 u_i}{\partial x_k \partial x_k} + u_j F_i, \tag{A.2}$$

and consider the same expression with i and j interchanged:

$$u_i \frac{\partial u_j}{\partial t} + u_i \frac{\partial}{\partial x_k}\left(u_j u_k\right) = -u_i \frac{\partial p}{\partial x_j} + \nu u_i \frac{\partial^2 u_j}{\partial x_k \partial x_k} + u_i F_j. \tag{A.3}$$

Adding (A.2) and (A.3) gives

$$\begin{aligned} \frac{\partial (u_i u_j)}{\partial t} + \frac{\partial}{\partial x_k}\left(u_i u_j u_k\right) = &- \left[\frac{\partial}{\partial x_j}(p u_i) + \frac{\partial}{\partial x_i}(p u_j) - p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] \\ &+ \nu\left(u_i \frac{\partial^2 u_j}{\partial x_k x_k} + u_j \frac{\partial^2 u_i}{\partial x_k x_k}\right) + u_i F_j + u_j F_i. \end{aligned} \tag{A.4}$$

Using

$$s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{A.5}$$

and

$$\frac{\partial^2 (u_i u_j)}{\partial x_k \partial x_k} = u_i \frac{\partial^2 u_j}{\partial x_k \partial x_k} + 2\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k} + u_j \frac{\partial^2 u_i}{\partial x_k \partial x_k}, \tag{A.6}$$

we obtain equation (3.23)

$$\begin{aligned} \frac{\partial (u_i u_j)}{\partial t} + \frac{\partial}{\partial x_k}\left(u_i u_j u_k\right) = &- \frac{\partial}{\partial x_k}\left[p u_i \delta_{jk} + p u_j \delta_{ik} - \nu \frac{\partial (u_i u_j)}{\partial x_k}\right] + 2 p s_{ij} \\ &- 2\nu \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k} + u_i F_j + u_j F_i. \end{aligned} \tag{A.7}$$

Operating on this with a filter:

$$\begin{aligned}\frac{\partial\langle u_iu_j\rangle}{\partial t}+\frac{\partial}{\partial x_k}\langle u_iu_ju_k\rangle =&-\frac{\partial}{\partial x_k}\left[\langle pu_i\rangle\delta_{jk}+\langle pu_j\rangle\delta_{ik}-\nu\frac{\partial\langle u_iu_j\rangle}{\partial x_k}\right]+2\langle ps_{ij}\rangle\\&-2\nu\left\langle\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}\right\rangle+\langle u_iF_j\rangle+\langle u_jF_i\rangle.\end{aligned}\tag{A.8}$$

Writing the filtered momentum equation (2.33) in the same form as (A.1):

$$\frac{\partial\langle u_i\rangle}{\partial t}+\frac{\partial}{\partial x_k}\left(\langle u_i\rangle\langle u_k\rangle\right)=-\frac{\partial\langle p\rangle}{\partial x_i}+\nu\frac{\partial^2\langle u_i\rangle}{\partial x_k\partial x_k}+\langle F_i\rangle-\frac{\partial}{\partial x_k}(\tau(u_i,u_k)).\tag{A.9}$$

By the same approach as above, we obtain

$$\begin{aligned}&\frac{\partial(\langle u_i\rangle\langle u_j\rangle)}{\partial t}+\frac{\partial}{\partial x_k}\left(\langle u_i\rangle\langle u_j\rangle\langle u_k\rangle\right)\\&\qquad=-\frac{\partial}{\partial x_k}\left[\langle p\rangle\langle u_i\rangle\delta_{jk}+\langle p\rangle\langle u_j\rangle\delta_{ik}-\nu\frac{\partial(\langle u_i\rangle\langle u_j\rangle)}{\partial x_k}\right]\\&\qquad\quad+2\langle p\rangle\langle s_{ij}\rangle-2\nu\frac{\partial\langle u_i\rangle}{\partial x_k}\frac{\partial\langle u_j\rangle}{\partial x_k}+\langle u_i\rangle\langle F_j\rangle+\langle u_j\rangle\langle F_i\rangle-T_{ij},\end{aligned}\tag{A.10}$$

where

$$T_{ij}=\langle u_i\rangle\frac{\partial}{\partial x_k}(\tau(u_j,u_k))+\langle u_j\rangle\frac{\partial}{\partial x_k}(\tau(u_i,u_k)),\tag{A.11a}$$

$$=\frac{\partial}{\partial x_k}\left[\langle u_i\rangle\tau(u_j,u_k)+\langle u_j\rangle\tau(u_i,u_k)\right]-\frac{\partial\langle u_i\rangle}{\partial x_k}\tau(u_j,u_k)-\frac{\partial\langle u_j\rangle}{\partial x_k}\tau(u_i,u_k).\tag{A.11b}$$

Subtracting (A.10) from (A.8) then gives

$$\begin{aligned}&\frac{\partial(\tau(u_i,u_j))}{\partial t}+\frac{\partial}{\partial x_k}\left[\langle u_iu_ju_k\rangle-\langle u_i\rangle\langle u_j\rangle\langle u_k\rangle\right]\\&\qquad=-\frac{\partial}{\partial x_k}\left[\tau(p,u_i)\delta_{jk}+\tau(p,u_j)\delta_{ik}-\nu\frac{\partial(\tau(u_i,u_j))}{\partial x_k}\right]+2\tau(p,s_{ij})\\&\qquad\quad-2\nu\tau\left(\frac{\partial u_i}{\partial x_k},\frac{\partial u_j}{\partial x_k}\right)+\tau(u_i,F_j)+\tau(u_j,F_i)+T_{ij}.\end{aligned}\tag{A.12}$$

Comparing (A.11b) with the definition of the generalised third moment

$$\begin{aligned}\tau(u_i,u_j,u_k)=&\langle u_iu_ju_k\rangle-\langle u_i\rangle\tau(u_j,u_k)-\langle u_j\rangle\tau(u_k,u_i)\\&-\langle u_k\rangle\tau(u_i,u_j)-\langle u_i\rangle\langle u_j\rangle\langle u_k\rangle,\end{aligned}\tag{A.13}$$

we can rearrange (A.12) and cancel terms to obtain equation (3.24)

$$\begin{aligned}\frac{\partial\tau(u_i,u_j)}{\partial t}+\frac{\partial}{\partial x_k}\left(\tau(u_i,u_j)\langle u_k\rangle\right)=&-\frac{\partial}{\partial x_k}\Big\{\tau(u_i,u_j,u_k)+\tau(p,u_i)\delta_{jk}\\&+\tau(p,u_j)\delta_{ik}-\nu\frac{\partial\tau(u_i,u_j)}{\partial x_k}\Big\}\\&+2\tau(p,s_{ij})-2\nu\tau\left(\frac{\partial u_i}{\partial x_k},\frac{\partial u_j}{\partial x_k}\right)\\&-\tau(u_i,u_k)\frac{\partial\langle u_j\rangle}{\partial x_k}-\tau(u_j,u_k)\frac{\partial\langle u_i\rangle}{\partial x_k}\\&+\tau(u_i,F_j)+\tau(u_j,F_i).\end{aligned}\tag{A.14}$$

Contracting this equation with δ_{ij} and halving gives an equation for $E_T = \frac{1}{2}\tau(u_i, u_i)$:

$$\begin{aligned}\frac{\partial E_T}{\partial t} + \frac{\partial (E_T \langle u_k \rangle)}{\partial x_k} = &- \frac{\partial}{\partial x_k}\left[\frac{1}{2}\tau(u_i, u_i, u_k) + \tau(p, u_k) - \nu \frac{\partial E_T}{\partial x_k}\right] \\ &- \nu\tau\left(\frac{\partial u_i}{\partial x_k}, \frac{\partial u_i}{\partial x_k}\right) - \tau(u_i, u_k)\frac{\partial \langle u_i \rangle}{\partial x_k} + \tau(u_i, F_i).\end{aligned} \tag{A.15}$$

We rewrite the penultimate term by taking the filter outside the spatial derivative and decomposing the velocity gradient into symmetric and anti-symmetric parts:

$$\tau(u_i, u_k)\frac{\partial \langle u_i \rangle}{\partial x_k} = \tau(u_i, u_k)\left\langle \frac{\partial u_i}{\partial x_k} \right\rangle, \tag{A.16a}$$

$$= \tau(u_i, u_k)\left\langle \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right) + \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} - \frac{\partial u_k}{\partial x_i}\right)\right\rangle. \tag{A.16b}$$

The last term in the angle brackets $\langle \cdot \rangle$ is anti-symmetric, and is contracted with $\tau(u_i, u_k)$ which is symmetric, so the last term vanishes, leaving

$$\tau(u_i, u_k)\frac{\partial \langle u_i \rangle}{\partial x_k} = \tau(u_i, u_k)\langle s_{ij} \rangle. \tag{A.17}$$

Substituting (A.17) into (A.15) leads to equation (3.26):

$$\begin{aligned}\frac{\partial E_T}{\partial t} + \frac{\partial (E_T \langle u_k \rangle)}{\partial x_k} = &- \frac{\partial}{\partial x_k}\left[\frac{1}{2}\tau(u_i, u_i, u_k) + \tau(p, u_k) - \nu \frac{\partial E_T}{\partial x_k}\right] \\ &- \nu\tau\left(\frac{\partial u_i}{\partial x_k}, \frac{\partial u_i}{\partial x_k}\right) - \tau(u_i, u_k)\langle s_{ik} \rangle + \tau(u_i, F_i).\end{aligned} \tag{A.18}$$

Appendix B

Gramian Matrices Proof

In section 3.3, we proved that the subgrid tensor $\boldsymbol{\tau}$ is positive semidefinite if and only if the filter kernel G is positive everywhere. Our proof used the result that every Gramian matrix is positive semidefinite, which is proved in this appendix.

For a set of vectors $\{v_1, v_2, v_3\}$ in a 3-dimensional vector space V, the Gramian matrix A is defined as having entries

$$a_{ij} = [v_i, v_j], \qquad i, j \in \{1, 2, 3\} \tag{B.1}$$

where $[\,\cdot\,,\,\cdot\,]$ is an inner product on V.

We want to show that any Gramian matrix satisfies the realizability conditions (3.30) to (3.32) as repeated below:

$$a_{ii} \geq 0, \qquad \text{for} \quad i \in \{1, 2, 3\}, \tag{B.2}$$

$$|a_{ij}| \leq \sqrt{a_{ii} a_{jj}}, \qquad \text{for} \quad i, j \in \{1, 2, 3\}, \tag{B.3}$$

$$\det A \geq 0. \tag{B.4}$$

By positivity of the inner product,

$$a_{ii} = [v_i, v_i] \geq 0 \quad \text{for all } i, \tag{B.5}$$

so (3.30) is immediately satisfied. The inner product also naturally defines a norm on V:

$$\|v_i\| = \sqrt{[v_i, v_i]}. \tag{B.6}$$

With this definition, we can apply the Cauchy–Schwarz inequality to obtain property (3.31)

$$|a_{ij}| = |[v_i, v_j]| \leq \|v_i\| \|v_j\| = \sqrt{[v_i, v_i][v_j, v_j]} = \sqrt{a_{ii} a_{jj}}. \tag{B.7}$$

Finally, we can use the inner product with Gram–Schmidt orthogonalisation (see Kaye & Wilson (1998)) to form an orthonormal basis $\{u_1, u_2, u_3\}$ for V. We can now express A as

$$A = M^T M \quad \text{where} \quad M = \begin{pmatrix} [v_1, u_1] & [v_2, u_1] & [v_3, u_1] \\ [v_1, u_2] & [v_2, u_2] & [v_3, u_2] \\ [v_1, u_3] & [v_2, u_3] & [v_3, u_3] \end{pmatrix}. \tag{B.8}$$

Then, since $\det(M^T) = \det M$,

$$\det A = (\det M)^2 \geq 0. \tag{B.9}$$

Therefore, any Gramian matrix is positive semidefinite.

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