2

LES Governing Equations

This chapter is divided in five main parts. The first one is devoted to the presentation of the chosen set of equations. The second part deals with the filtering paradigm and its peculiarities in the framework of compressible flows. In particular the question of discontinuities is addressed and the Favre filtering is introduced. Since the formulation of the energy equation is not unique, the third part first presents different popular formulations. Physical assumptions which permit a simplification of the system of equations are discussed. Furthermore, additional relationships relevant to LES modeling are introduced. Finally, in the last part, fundamentals of LES modeling are established and the distinction of the models according to functional and structural approaches is introduced.

2.1 Preliminary Discussion

Large-eddy simulation relies on the idea that some scales of the full turbulent solutions are discarded to obtain a desired reduction in the range of scales required for numerical simulation. More precisely, small scales of the flow are supposed to be more universal (according to the celebrated local isotropy hypothesis by Kolmogorov) and less determined by boundary conditions than the large ones in most engineering applications. Very large scales are sometimes also not directly represented during the computation, their effect must also be modeled. This mesoscale modeling is popular in the field of meteorology and oceanography. Let us first note here that small and large scales are not well defined concepts, which are flow dependent and not accurately determined by the actual theory of LES.

In practice, as all simulation techniques, LES consists of solving the set of governing equations for fluid mechanics (usually the Navier–Stokes equations, possibly supplemented by additional equations) on a discrete grid, i.e. using a finite number of degrees of freedom. The essential idea is that the spatial distribution of the grid nodes implicitly generates a scale separation, since

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scales smaller than a typical scale associated to the grid spacing cannot be captured. It is also worthy noting that numerical schemes used to discretize continuous operators, because they induce a scale-dependent error, introduce an additional scale separation between well resolved scales and poorly resolved ones.

As a consequence, the LES problem make several subranges of scales appearing:

- *represented resolved scales*, which are scales large enough to be accurately captured on the grid with a given numerical method.
- *represented non-resolved scales*, which are scales larger than the mesh size, but which are corrupted by numerical errors. These scales are the smallest represented scales.
- *non-represented scales*, i.e. scales which are too small to be represented on the computational grid.

One of the open problem in the field of LES is to understand and model the existence of these three scale subranges and to write governing equations for them. To address the modeling problem, several mathematical models for the derivation of LES governing equations have been proposed since Leonard in 1973, who introduced the filtering concept for removing small scales to LES.

The filtering concept makes it possible to address some problems analytically, including the closure problem and the definition of boundary conditions. One the other hand the filtering concept introduces some artefacts, i.e. conceptual problems which are not present in the original formulation. An example is the commutation error between the convolution filter and a discretization scheme.

The most popular filter concept found in the literature for LES of compressible flows is the convolution filter approach, which will be extensively used hereafter. Several other concepts have been proposed for incompressible flow simulation, the vast majority of which having not been extended to compressible LES.

2.2 Governing Equations

2.2.1 Fundamental Assumptions

The framework is restricted to compressible gas flows where the continuum hypothesis is valid. This implies that the chosen set of equations will be derived in control volumes that will be large enough to encompass a sufficient number of molecules so that the concept of statistical average hold. The behavior of the fluid can then be described by its macroscopic properties such as its pressure, its density and its velocity. Even if one can expect that the Knudsen number (ratio of the mean free path of the molecules over a characteristic dimension of the flow) be of the order of 1 in shocks, Smits and Dussauge [266] notice that for shocks of reasonable intensity (where the shock thickness is of the order of few mean free paths) the continuum equations for the gas give shock structure in agreement with experiments.

For sake of simplicity, we consider only gaseous fluid: multi-phase flows are not considered. Furthermore, we restrict our discussion to non-reactive mono-species gases. With respect to issues related to combustion the reader may consult Ref. [220]. Moreover, the scope of this monograph is restricted to non-hypersonic flows (Mach < 6 in air) for which dissociation and ionization effects occurring at the molecular level can be neglected. Temperature differences are supposed to be sufficiently weak so that radiative heat transfer can be neglected. Furthermore, a local thermodynamic equilibrium is assumed to hold everywhere in the flow. With the aforementioned assumptions a perfect gas equation of state can be employed. We restrict ourselves to Newtonian fluids for which the dynamic viscosity varies only with temperature. Since we consider non-uniform density fields, gravity effects could appear. Nevertheless, the Froude number which describes the significance of gravity effects as computed to inertial effects is assumed to be negligible regarding the high velocity of the considered flows (Mach > 0.2).

Finally, the compressible Navier-Stokes equations which express the conservation of mass, momentum, and energy are selected as a mathematical model for the fluids considered in this textbook. These differential equations are supplemented by an algebraic equation, the perfect gas equation of state.

2.2.2 Conservative Formulation

The way the energy conservation is expressed in the Navier-Stokes equations is not unique. Formulations exist for the temperature, pressure, enthalpy, internal energy, total energy, and entropy. Nevertheless, the only way to formulate this equation in conservative form is to chose the total energy. The conservative formulation is necessary for capturing possible discontinuities of the flow at the correct velocity in numerical simulations [155].

Using this form, the Navier-Stokes equations can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2.2}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p) u_j}{\partial x_j} = \frac{\partial \sigma_{ij} u_i}{\partial x_j} - \frac{\partial}{\partial x_j} q_j, \tag{2.3}$$

where t and x_i are independent variables representing time and spatial coordinates of a Cartesian coordinate system $\mathbf{x}$, respectively. The three components of the velocity vector $\mathbf{u}$ are denoted u_i $(i = 1, 2, 3)$. The summation convention over repeated indices applies. The total energy per mass unit E is given by:

$$\rho E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u_i u_i \tag{2.4}$$

and the density ρ, the pressure p and the static temperature T are linked by the equation of state:

$$p = \rho R T. \tag{2.5}$$

The gas constant is $R = C_p - C_v$ where C_p and C_v are the specific heats at constant pressure and constant volume, respectively. The variation of these specific heats with respect to temperature is very weak and should not be taken into account according to the framework defined in the previous section. For air, R is equal to 287.03 $\mathrm{m}^2\,\mathrm{s}^2\,\mathrm{K}$.

According to the Stokes's hypothesis which assumes that the bulk viscosity can be neglected, the shear-stress tensor for a Newtonian fluid is given by:

$$\sigma_{ij} = 2\mu(T) S_{ij} - \frac{2}{3}\mu(T)\delta_{ij} S_{kk}, \tag{2.6}$$

where S_{ij}, the components of rate-of-strain tensor $S(\mathbf{u})$ are written as:

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{2.7}$$

The variation of the dynamic viscosity μ with temperature can be accounted for by the Sutherland's law

$$\frac{\mu(T)}{\mu(T_0)} = \left(\frac{T}{T_0}\right)^{\frac{3}{2}} \frac{T_0 + S_1}{T + S_1}, \quad \text{with } S_1 = 110.4 \text{ K} \tag{2.8}$$

which is valid from 100 K to 1900 K [266]. It is often approximated by the power law

$$\frac{\mu(T)}{\mu(T_0)} = \left(\frac{T}{T_0}\right)^{0.76}, \tag{2.9}$$

which is valid between 150 K and 500 K. The use of these laws introduces an additional non-linearity in the momentum and energy equations.

The heat flux q_j is given by

$$q_j = -\kappa \frac{\partial T}{\partial x_j}, \tag{2.10}$$

where κ is the thermal conductivity which can be expressed as $\kappa = \mu C_p / Pr$. The Prandtl number is the ratio of the kinematic viscosity $\nu = \mu/\rho$ and thermal diffusivity $\kappa/(\rho C_p)$ and, is assumed to be constant equal to 0.72 for air.

2.2.3 Alternative Formulations

Four alternative formulations have been employed in the literature for LES of compressible flows.

The enthalpy form has been used by Erlebacher et al. [75]

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_j}{\partial x_j} = \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial}{\partial x_j} T\right) + \Phi, \tag{2.11}$$

where the enthalpy $h = C_p T$, and the viscous dissipation Φ is defined as:

$$\Phi = \sigma_{ij} \frac{\partial u_i}{\partial x_j}. \tag{2.12}$$

It can be noted that this form includes the temporal derivative of the pressure on the right hand side.

The temperature form has been used by Moin et al. [201]. As the following pressure form, it corresponds to an equation for the internal energy $\epsilon = C_v T$

$$\frac{\partial}{\partial t}(\rho C_v T) + \frac{\partial}{\partial x_j}(\rho u_j C_v T) = -p \frac{\partial u_j}{\partial x_j} + \Phi + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right). \tag{2.13}$$

The pressure form can be found in the work by Zang et al. [323]

$$\frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \gamma p \frac{\partial u_j}{\partial x_j} = (\gamma - 1)\Phi + (\gamma - 1)\frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right), \tag{2.14}$$

where $\gamma = C_p/C_v$. Its value is fixed to 1.4 for air according to the aforementioned framework.

The entropy form has been employed by Mathew et al. [194].

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \rho s u_j}{\partial x_j} = \frac{1}{T}\left[\Phi + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\right], \tag{2.15}$$

with $s = C_v \ln(p\rho^{-\gamma})$.

2.3 Filtering Operator

Large-eddy simulation is based on the idea of scale separation or filtering with a mathematically well-established formalism. We restrict our presentation here to the fundamental definitions. The entire formalism can be found in Ref. [244]. The specifics for compressible flows such as the notion of filtering of discontinuous flows and the Favre variables are detailed.

2.3.1 Definition

The framework of this section is restricted to the ideal case of homogeneous turbulence. This implies that the filter should respect the physical properties of isotropy and homogeneity. Subsequently, the filter properties are independent of the position and of the orientation of the frame of reference in space. As a result, its cut-off scale is constant and identical in all spatial directions. To address the issue of discontinuous flows, non-centered filters which are not isotropic may be defined. We put the emphasis on isotropic filters on which LES is grounded. Reference [244] provides an extension to inhomogeneous filters.

Scales are separated using a scale high-pass filter which is also a low-pass filter in frequency. Filtering is represented mathematically in physical space as a convolution product. The resolved part $\bar{\phi}(\mathbf{x},t)$ of a space-time variable $\phi(\mathbf{x},t)$ is defined formally by the relation

$$\bar{\phi}(\mathbf{x},t) = \frac{1}{\Delta}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G\left(\frac{\mathbf{x}-\boldsymbol{\xi}}{\Delta}, t-t'\right)\phi(\xi,t')dt'd^3\boldsymbol{\xi}, \tag{2.16}$$

where the convolution kernel G is characteristic of the filter used, and is associated with the cut-off scale in space and time, Δ and τ_c, respectively. This relation is denoted symbolically by

$$\bar{\phi} = G \star \phi. \tag{2.17}$$

The dual definition in Fourier space is obtained by multiplying the spectrum $\hat{\phi}(\mathbf{k},\omega)$ of $\phi(\mathbf{x},t)$ by the transfer function $\hat{G}(\mathbf{k},\omega)$ of the kernel $G(\mathbf{x},t)$:

$$\bar{\hat{\phi}}(\mathbf{k},\omega) = \hat{G}(\mathbf{k},\omega)\hat{\phi}(\mathbf{k},\omega), \tag{2.18}$$

or in symbolic form

$$\bar{\hat{\phi}} = \hat{G}\hat{\phi}, \tag{2.19}$$

where $\mathbf{k}$ and ω are wave number and frequency, respectively. The spatial cutoff length Δ is associated to the cutoff wave number k_c and time τ_c with the cutoff frequency ω_c.

The non-resolved part of $\phi(\mathbf{x},t)$, denoted $\phi'(\mathbf{x},t)$ is defined as:

$$\phi'(\mathbf{x},t) = \phi(\mathbf{x},t) - \bar{\phi}(\mathbf{x},t), \tag{2.20}$$

or

$$\phi' = (1-G)\star\phi. \tag{2.21}$$

Fundamental Properties

For further manipulating of the Navier-Stokes equations after filter application, we require the following three properties:

- Consistency
$$\bar{a} = a \longleftrightarrow \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G(\boldsymbol{\xi}, t')d^3\boldsymbol{\xi}dt' = 1. \tag{2.22}$$
- Linearity
$$\overline{\phi + \psi} = \bar{\phi} + \bar{\psi} \tag{2.23}$$
which is satisfied by the convolution form of filtering.
- Commutation with differentiation[1]
$$\overline{\frac{\partial \phi}{\partial s}} = \frac{\partial \bar{\phi}}{\partial s}, \quad s = \mathbf{x}, t \tag{2.24}$$

Introducing the commutator $[f, g]$ of two operators f and g applied to a dummy variable ϕ
$$[f, g](\phi) = f \circ g(\phi) - g \circ f(\phi) = f\left(g(\phi)\right) - g\left(f(\phi)\right) \tag{2.25}$$
the relation (2.24) can be rewritten as
$$\left[G\star, \frac{\partial}{\partial s}\right] = 0. \tag{2.26}$$
This commutator satisfies the Leibniz identity
$$[f \circ g, h] = [f, h] \circ g + f \circ [g, h]. \tag{2.27}$$

The filter G is not *a priori* a Reynolds operator, since the following property of this kind of operator is not satisfied in general
$$\overline{\phi\bar{\psi}} = \bar{\phi}\bar{\psi}. \tag{2.28}$$
The filter $\overline{(.)}$ is not necessarily idempotent (i.e. G is not a projector), and the large scale component of a fluctuating quantity does not vanish
$$\bar{\bar{\phi}} = G \star G \star \phi = G^2\phi \neq \bar{\phi}, \tag{2.29}$$
$$\overline{\phi'} = G \star (1 - G) \star \phi \neq 0. \tag{2.30}$$
Let us note that some filter can be inverted, leading to the preservation of the information present in the full exact solution. Conversely, if the filter is a Reynolds operator, the inversion is no longer possible since its kernel $ker(G) = \phi'$ is no longer reduced to the zero element. In this case, the filtering induces an irremediable loss of information.

[1] The space commutation property is satisfied only if the domain is unbounded and if the convolution kernel is homogeneous (Δ constant and independent of space). It is however necessary to vary the cut-off length in order to adapt it to the structure of the solution. For example, this adaptation is mandatory for wall-bounded flows for which the filter length scale must diminish close to the wall in order to capture the smallest dynamically active scales. Ghosal and Moin [96] have shown for the case of homogeneous filters that the commutation error is not bounded. They propose a method to guarantee a second-order commutation error. More recently, Vasilyev et al. [299] have defined filters commuting at an arbitrarily high order.

Additional Hypothesis

The framework presented above is very general. In practice, additional constraints are needed. We now assume that the space-time convolution kernel $G(\mathbf{x}-\boldsymbol{\xi}, t-t')$ is obtained by tensorial extension of one-dimensional kernels

$$G\left(\frac{\mathbf{x}-\boldsymbol{\xi}}{\Delta}, t-t'\right) = G_t(t-t')G\left(\frac{\mathbf{x}-\boldsymbol{\xi}}{\Delta}\right) = G_t(t-t')\prod_{i=1,3} G_i\left(\frac{x_i-\xi_i}{\Delta}\right). \tag{2.31}$$

Since up to now there is no example of LES of compressible flow based on temporal filtering, we restrict our discussion to spatial filtering. Mathematically, this additional restriction is expressed by

$$G_t(t-t') = \delta(t-t'). \tag{2.32}$$

Nevertheless, one has to keep in mind that the spatial filtering implies a temporal filtering since the dynamics of the Navier-Stokes equations make it possible to associate a characteristic time scale with a length scale. The latter one, denoted t_c following dimensional argument can be computed as

$$t_c = \Delta/\sqrt{k_c E(k_c)}, \tag{2.33}$$

where $k_c E(k_c)$ is the kinetic energy associated to the cutoff wave number $k_c = \pi/\Delta$. Suppressing the spatial scales corresponding to wave numbers higher than k_c implies the suppression of frequencies higher than the cutoff frequency $\omega_c = 2\pi/t_c$.

Three Classical Filters for Large Eddy Simulation

Three particular convolution filters are commonly used for performing the spatial scale separation, the Box or top hat filter, the Gaussian filter, and the spectral or sharp cutoff filter. Their kernel functions are given in Table 2.1 both in physical and spectral space for one spatial dimension. The parameter ς of the Gaussian filter is generally taken equal to 6. Both Gaussian and Box filters have a compact support in physical space.

Table 2.1. Kernels of three classical filters

Filter	Kernel in physical space G	Kernel in spectral space $\hat{G}$
Box filter	$G(x-\xi) = \begin{cases} \frac{1}{\Delta} & \text{if} \lvert x-\xi\rvert \le \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases}$	$\hat{G}(k) = \frac{\sin(k\Delta/2)}{k\Delta/2}$
Gaussian	$G(x-\xi) = (\frac{\varsigma}{\pi\Delta^2})^{1/2}\exp(\frac{-\varsigma(x-\xi)^2}{\Delta^2})$	$\hat{G}(k) = e^{-(\Delta^2 k^2)/4\varsigma}$
Sharp cutoff	$G(x-\xi) = \frac{\sin(k_c(x-\xi))}{k_c(x-\xi)}$ with $k_c = \frac{\pi}{\Delta}$	$\hat{G}(k) = \begin{cases} 1 & \text{if } \lvert k\rvert < k_c \\ 0 & \text{otherwise} \end{cases}$

Differential Interpretation of the Filters

For filters defined on the compact support $[\Delta\alpha, \Delta\beta]$ (with $\alpha \neq \beta$), the following definition of filtering can be adopted in the one-dimensional case:

$$\bar{\phi}(x,t) = \frac{1}{\Delta}\int_{x-\Delta\beta}^{x-\Delta\alpha} G\left(\frac{x-\xi}{\Delta}\right)\phi(\xi,t)d\xi \tag{2.34}$$

$$= \int_{\alpha}^{\beta} G(z)\phi(x-\Delta z,t)dz \tag{2.35}$$

In order to facilitate the following developments, the change of variable $z = (x-\xi)/\Delta$ was employed to derive (2.35) from (2.34).

To go toward a differential interpretation of the filter, we perform a Taylor series expansion of the $\phi(\xi,t)$ term at (x,t):[2]

$$\phi(\xi,t) = \phi(x,t) + \sum_{l=1}^{\infty}\frac{(\xi-x)^l}{l!}\frac{\partial^l\phi(x,t)}{\partial x^l}. \tag{2.36}$$

With the aforementioned change of variable, equation (2.36) can be recast as

$$\phi(x-\Delta z,t) = \phi(x,t) + \sum_{l=1}^{\infty}\frac{(-1)^l(\Delta z)^l}{l!}\frac{\partial^l\phi(x,t)}{\partial x^l}, \tag{2.37}$$

Introducing this expansion into (2.35) and considering the symmetry and the conservation properties of the constants of the kernel G, we get

$$\begin{aligned}\bar{\phi}(x,t) &= \int_{\alpha}^{\beta} G(z)\phi(x,t)dz + \int_{\alpha}^{\beta}\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\Delta^l z^l G(z)\frac{\partial^l\phi(x,t)}{\partial x^l}dz \\ &= \phi(x,t) + \sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\Delta^l M_l\frac{\partial^l\phi(x,t)}{\partial x^l}\end{aligned} \tag{2.38}$$

where M_l is the lth-order moment of the convolution kernel

$$M_l = \int_{\alpha}^{\beta} z^l G(z)dz \tag{2.39}$$

Odd moments vanish for a centered kernel. The differential form (2.38) is well posed if and only if $\forall l\ |M_l| < \infty$ meaning that the kernel G decays rapidly in space. The first five non zero moments for both box and Gaussian filters are given in Table 2.2.

[2] This implies that the turbulent field is smooth enough so that a Taylor series expansion exists.

Table 2.2. Values of the first five non-zero moments for the Box and Gaussian filters

M_l	$l=0$	$l=2$	$l=4$	$l=6$	$l=8$
Box	1	1/12	1/80	1/448	1/2304
Gaussian	1	1/12	1/48	5/576	35/6912

2.3.2 Discrete Representation of Filters

From practical considerations, the filter must be expressed in a discrete form. The filtered field at the ith grid point $\bar{\phi}_i$ obtained by applying a discrete filter with a $(M+N+1)$ points stencil to the variable ϕ, is formally defined on a uniform grid with mesh size Δx as

$$\bar{\phi}_i = G\phi_i = \sum_{n=-M}^{N} a_n \phi_{i+n}. \tag{2.40}$$

where the real coefficients a_n specify the filter. The preservation of a constant variable is ensured under the condition

$$\sum_{n=-M}^{N} a_n = 1 \tag{2.41}$$

The transfer function of this filter kernel can be expressed as

$$\hat{G}(k) = \sum_{n=-M}^{N} a_n e^{jkn\Delta x}, \quad \text{with } j^2 = -1. \tag{2.42}$$

Introducing the Taylor series for each n

$$\phi_{i\pm n} = \sum_{l=0}^{\infty} \frac{(\pm n\Delta x)^l}{l!} \frac{\partial^l \phi}{\partial x^l}, \tag{2.43}$$

gives on substitution into (2.40)

$$\bar{\phi}_i = \sum_{n=-M}^{N} a_n \sum_{l=0}^{\infty} \frac{n^l \Delta x^l}{l!} \frac{\partial^l \phi}{\partial x^l}, \tag{2.44}$$

which can be recast as

$$\bar{\phi}_i = \left(1 + \sum_{l=1}^{\infty} a_n^* \Delta x^l \frac{\partial^l}{\partial x^l}\right) \phi_i. \tag{2.45}$$

where we have introduced the abbreviation

$$a_n^* = \frac{1}{l!} \sum_{n=-M}^{N} a_n n^l. \tag{2.46}$$

Additionally, (2.38) can be recast by virtue of the parameter $\epsilon = \Delta/\Delta x$ which represents the ratio of the mesh size Δx to the cut-off length scale Δ, as

$$\bar{\phi}(x,t) = \phi(x,t) + \sum_{l=1}^{\infty} \frac{(-1)^l}{l!} (\epsilon \Delta x)^l M_l \frac{\partial^l \phi(x,t)}{\partial x^l}. \tag{2.47}$$

The a_n are obtained as solution of a linear system which results from computing terms of like order in (2.47) and (2.45).

As an example, using the values of the moments M_l provided in Table 2.2 up to $l = 4$, the fourth-order approximation of the Gaussian filter is

$$\bar{\phi}_i = \frac{\epsilon^4 - 4\epsilon^2}{1152} \left(\phi_{i+2} + \phi_{i-2}\right) + \frac{16\epsilon^2 - \epsilon^4}{288} \left(\phi_{i+1} + \phi_{i-1}\right) + \frac{\epsilon^4 - 20\epsilon^2 + 192}{192} \phi_i. \tag{2.48}$$

Up to second order, the approximation of Box and Gaussian filters is identical, and for $\epsilon = \sqrt{6}$, one can derive the very popular three-point symmetric filter

$$\bar{\phi}_i = \frac{1}{4}(\phi_{i-1} + 2\phi_i + \phi_{i+1}). \tag{2.49}$$

The Simpson integration rule can be applied with $\epsilon = 2$ to obtain

$$\bar{\phi}_i = \frac{1}{6}(\phi_{i-1} + 4\phi_i + \phi_{i+1}). \tag{2.50}$$

In order to ensure that derivation commutes with filtering, one can define high-order commuting filters that have vanishing moments up to an arbitrary order (for boundary conditions, non symmetric filters are considered) [299]. An additional constrain is added to ensure that the transfer function of the filter is null at the cut-off wave number $k_c = \pi/\Delta x$. In discrete form, this leads to

$$\hat{G}(k_c) = \sum_{n=-M}^{N} (-1)^n a_n = 0. \tag{2.51}$$

This kind of filters belongs to the category of linearly constrained filters [299]. Increasing the number of vanishing moments also allows to find a better approximation of a sharp cutoff filter.

Considering the particular case $N = M$, the complex transfer function (2.42) can be decomposed in real and imaginary parts:

$$\Re\{\hat{G}(k)\} = a_0 + \sum_{n=1}^{N} (a_n + a_{-n}) \cos(kn\Delta x), \tag{2.52}$$

$$\Im\{(\hat{G}(k)\} = \sum_{n=1}^{N} (a_n - a_{-n}) \sin(kn\Delta x), \tag{2.53}$$

The latter of which vanishes in the particular case on a symmetric filter ($a_n = a_{-n}$).

For optimal filters, these coefficients are computed as to minimize the functional

$$\int_0^{\pi/\Delta x} (\Re\{\hat{G}(k) - \hat{G}_{target}(k)\})^2 dk + \int_0^{\pi/\Delta x} (\Im\{\hat{G}(k) - \hat{G}_{target}(k)\})^2 dk \quad (2.54)$$

where $G_{target}(k)$ is the target transfer function. Such filters have been proposed by [240, 299].

Finally, implicit filters defined as

$$\sum_{n=-P}^{P} b_n \bar{\phi}_{i+n} = a_n \phi_{i+n}. \quad (2.55)$$

These are an important part of the Approximate Deconvolution Method [277] (see Chap. 5).

2.3.3 Filtering of Discontinuities

As remarked by Lele [165], for a shock wave occurring in a turbulent flow the classical jump conditions hold for the instantaneous flow. Sagaut and Germano [243] have noticed that the usual filtering procedures, based on a central spatial filter that provides information from both sides, when applied around the discontinuity, produce parasitic contributions that affect the filtered quantities. This issue is developed in the following. Let us consider an unsteady fluctuating variable ϕ defined in a region Ω. We consider the case where this variable oscillates around a mean value U_0 in the subdomain Ω_0 and around the mean value U_1 in the subdomain Ω_1, where $\Omega_0 \bigcup \Omega_1 = \Omega$. The two subdomains do not overlapp and have an interface Γ. Using this domain decomposition, we obtain

$$\phi(x,t) = \begin{cases} \phi_0(x,t) = U_0(t) + \varrho_0(x,t) & x \in \Omega_0, \\ \phi_1(x,t) = U_1(t) + \varrho_1(x,t) & x \in \Omega_1 \end{cases} \quad (2.56)$$

where ϱ_p, $p = 0, 1$ represent the "turbulent" contribution around the mean value U_p. We assume in the following for the sake of simplicity that the function G has a compact support denoted as $S(x)$ at point x, i.e.

$$G\left(\frac{x-\xi}{\Delta}\right) = 0 \quad \text{if } \xi \notin S(x). \quad (2.57)$$

Filter applied to $\phi(x,t)$ gives

$$\bar{\phi}(x,t) = \frac{1}{\Delta} \int_{\Omega} G\left(\frac{x-\xi}{\Delta}\right) \phi(\xi) d\xi \quad (2.58)$$

We assume a central filter, i.e. its kernel is isotropic. By combination of (2.56) and (2.58), we get the following expression for $\bar{\phi}(x,t)$

$$\begin{aligned}\bar{\phi}(x,t) &= \frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)(U_0+\varrho_0(\xi,t))d\xi \\ &\quad + \frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)(U_1+\varrho_1(\xi,t))d\xi \end{aligned} \tag{2.59}$$

$$\begin{aligned} &= U_0\frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)d\xi + \frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_0(\xi,t)d\xi \\ &\quad + U_1\frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)d\xi + \frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_1(\xi,t)d\xi \end{aligned} \tag{2.60}$$

$$\begin{aligned} &= \underbrace{[[U]]\,\frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)d\xi}_{I} + U_0 \\ &\quad + \underbrace{\frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_0(\xi,t)d\xi + \frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_1(\xi,t)d\xi}_{II} \end{aligned} \tag{2.61}$$

$$\begin{aligned} &= \underbrace{-\,[[U]]\,\frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)d\xi}_{III} + U_1 \\ &\quad + \underbrace{\frac{1}{\Delta}\int_{\Omega_0\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_0(\xi,t)d\xi + \frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G\left(\frac{x-\xi}{\Delta}\right)\varrho_1(\xi,t)d\xi}_{II} \end{aligned} \tag{2.62}$$

where the jump operator is defined as

$$[[U]] = U_1 - U_0. \tag{2.63}$$

It can be seen that terms I and III in relations (2.61) and (2.62) are not related to "turbulent" fluctuations ϱ_p, $p=0,1$, but only to the discontinuity in the mean field. A first look at these terms shows that the filtered variable $\bar{\phi}(x,t)$ is not discontinuous, the sharp interface having been smoothed to become a graded solution over a region of thickness $2R$, where R is the radius of the kernel support S. The subgrid fluctuation $\phi'(x,t) \equiv \phi(x,t) - \bar{\phi}(x,t)$ is therefore equal to

$$\phi'(x,t) = \begin{cases} \varrho_0(x,t) - (II) - [[U]]\frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G(\frac{x-\xi}{\Delta})d\xi & x\in\Omega_0, \\ \varrho_1(x,t) - (II) + [[U]]\frac{1}{\Delta}\int_{\Omega_1\cap S(x)} G(\frac{x-\xi}{\Delta})d\xi & x\in\Omega_1. \end{cases} \tag{2.64}$$

It is observed that the jump in the mean field appears as a contribution in the definition of the subgrid fluctuation, which is an artefact of the filtering procedure. In the case of shocks, the contribution of the jump in the fluctuation will dominate the turbulent part of the subgrid fluctuations in most practical applications, rendering subgrid models which rely explicitly on the assumption that the subgrid fluctuations are of turbulent nature as inadequate. Sagaut and Germano [243] have defined non-centered filters which should be used to avoid this unphysical effect.

2.3.4 Filter Associated to the Numerical Method

The accuracy of a numerical scheme is traditionally associated to the order of its truncation error. However, in the framework of LES where the kinetic energy spectrum spreads over a wide range of scales, it seems more appropriate to compute the spectral distribution of the truncation error which can be associated to the filter transfer function in the wavenumber space. The notion of effective (or modified) wave number can be introduced [301]. To this end, the effect of the discretization on a periodic function $e^{j\alpha x}$ for which the exact derivative is $j\alpha e^{j\alpha x}$ is studied.

Consider the approximation of the first derivative $\frac{\partial f}{\partial x}$ at the ith node of a uniform grid

$$\frac{\partial f(x)}{\partial x} \simeq \frac{1}{\Delta x} \sum_{l=-N}^{M} a_l f_{i+l}. \tag{2.65}$$

The Fourier transform of f can be defined as

$$\tilde{f}(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-j\alpha x} dx. \tag{2.66}$$

This transform is applied to both sides of (2.65)

$$j\alpha\tilde{f} \simeq \left(\frac{1}{\Delta x} \sum_{l=-N}^{M} a_l e^{j\alpha l \Delta x} \right) \tilde{f}. \tag{2.67}$$

The quantity

$$\bar{\alpha} = \frac{-j}{\Delta x} \sum_{l=-N}^{M} a_l e^{j\alpha l \Delta x} \tag{2.68}$$

is the modified wave number of the Fourier transform of the finite difference scheme (2.65).

For example, for a second-order accurate centered scheme ($a_1 = a_{-1} = 1/2$), one obtains

$$\bar{\alpha} = \frac{-j}{\Delta x} \left(\frac{1}{2} e^{j\alpha\Delta x} - \frac{1}{2} e^{-j\alpha\Delta x} \right) = \frac{\sin(\alpha\Delta x)}{\Delta x} \tag{2.69}$$

which is second order accurate for small values of α. More generally, for a centered scheme where N=M and $a_l = a_{-l}$, the modified wave number is real. Conversely, if $N \neq M$ or $a_l \neq a_{-l}$, $\bar{\alpha}$ is complex, its imaginary part being associated to the dissipative character of the scheme. This character is shared by every schemes that are able to capture the discontinuities susceptible to occur in compressible flows.

As noted in Ref. [246], the filter transfer function can be written as

$$\hat{G} = \frac{\bar{\alpha}}{\alpha}. \tag{2.70}$$

The convolution kernel of few classical centered schemes are represented in Fig. 2.1 using the general formulae given by Lele [166] for both explicit and implicit (compact) centered schemes up to $M = N = 3$. The spectral scheme is optimal since its kernel is equal to 1. For low order schemes, the errors are large even for small wave numbers (large scales).

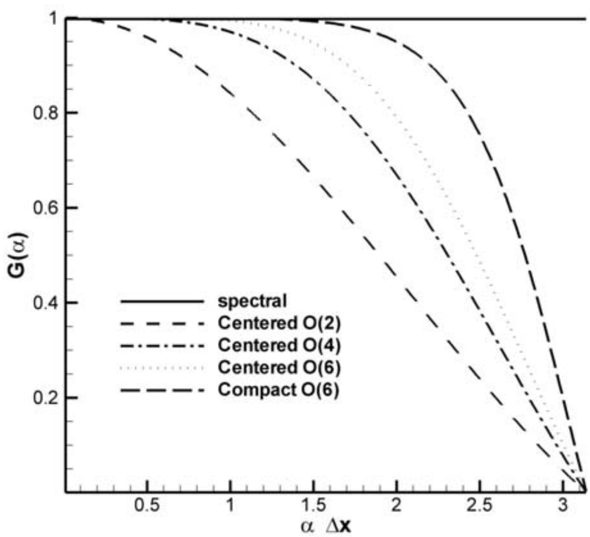

Fig. 2.1. Equivalent convolution kernel for some first order derivative schemes in Fourier space

Nevertheless, since the numerical schemes used are consistent, the numerical error cancels out as Δx tends towards zero. It is then possible to minimize the numerical error by employing a large $\Delta/\Delta x$ ratio. This technique, based on the decoupling of two length scales, is called pre-filtering and aims at ensuring the convergence of the solution regardless of the grid.[3]

[3] This technique is rarely used in practice since it leads to a simulation cost increased by a factor $(\Delta/\Delta x)^4$.

2.3.5 Commutation Error

Every product of two variables ϕ and ψ occurring in the Navier-Stokes equations give rise to a term $\overline{\phi\psi}$ whereas the computable variables are $\bar{\phi}$ and $\bar{\psi}$. Replacing $\overline{\phi\psi}$ by the product $\bar{\phi}\bar{\psi}$ introduces an error which is the commutation error between the filtering operator and the multiplication operator B defined by the bilinear form

$$B(a,b) = ab. \tag{2.71}$$

Using the commutator operator of (2.25), this error can be expressed as

$$\overline{\phi\psi} = \bar{\phi}\bar{\psi} + [G\star, B](\phi, \psi). \tag{2.72}$$

$[G\star, B](\phi, \psi)$ is a subgrid term since it takes account of information contained at subfilter scales. For incompressible flows, the commutation error implies the presence in the momentum equations of subgrid stress scale tensor defined as

$$[G\star, B](u_i, u_j) = \overline{u_i u_j} - \bar{u}_i \bar{u}_j. \tag{2.73}$$

The main modeling effort of the LES community has been concentrated on this term which is the only one arising for the incompressible equations for single phase flows.

2.3.6 Favre Filtering

Most authors dealing with LES of compressible flows have used a change of variable in which filtered variables are weighted by the density.[4] Mathematically, this change of variables is written as

$$\overline{\rho\phi} = \bar{\rho}\tilde{\phi}. \tag{2.74}$$

Any scalar or vector variable can be decomposed into a low frequency part $\tilde{\phi}$ and a high frequency part ϕ''

$$\phi = \tilde{\phi} + \phi''. \tag{2.75}$$

The $(\tilde{.})$ operator is linear but does not commute with the derivative operators in space and time

[4] To our knowledge, the classical LES filtering in compressible flows has been employed by Yoshizawa [320] and Bodony and Lele [23]. In Ref. [320], the analysis of compressible shear flows, realized with the aid of a multiscale Direct-Interaction Approximation, has been limited to weakly compressible flows. In Ref. [23] a simplified set of equations has been employed to compute cold and heated jets at Mach numbers ranging from 0.5 to 1.5. The merit of using the classical LES filtering is not discussed.

$$\widetilde{\frac{\partial \phi}{\partial x_j}} \neq \frac{\partial \tilde{\phi}}{\partial x_j}, \tag{2.76}$$

$$\widetilde{\frac{\partial \phi}{\partial t}} \neq \frac{\partial \tilde{\phi}}{\partial t}. \tag{2.77}$$

If the $\overline{(.)}$ operator is a Reynolds operator, the following relations can be established

$$\overline{\rho\phi''} = 0, \tag{2.78}$$

$$\bar{\phi} - \tilde{\phi} = \overline{\phi''} = -\frac{\overline{\rho'\phi'}}{\bar{\rho}} = -\frac{\overline{\rho'\phi''}}{\bar{\rho}}. \tag{2.79}$$

One can note the similarity of this change of variable with Favre [81] averaging. It is called "Favre filtering", keeping in mind that it is in fact a filtering expressed in terms of Favre variables by a change of variable.

The motivation of using such an operator is twofold:

- The term $\overline{\rho u_i}$ present in the filtered continuity equation can be decomposed following equation (2.72)

$$\overline{\rho u_i} = \bar{\rho}\,\overline{u_i} + [G\star, B](\rho, u_i) = \bar{\rho}\tilde{u}_i. \tag{2.80}$$

  With the filtering defined as in Sect. 2.3.1, the necessary transformation from $\overline{\rho u_i}$ to $\bar{\rho}\,\overline{u_i}$ would lead to another subgrid term which can be avoided by the change of variable (2.74) transforming $\overline{\rho u_i}$ to $\bar{\rho}\tilde{u}_i$.
- The "Favre-filtered" equations are structurally similar to their corresponding non filtered equations (with the exception of the subgrid terms). Moreover, in the framework of a RANS/LES coupling, the similarity with RANS equations can be beneficial. Generally, introducing the operator

$$H(a, b, c) = bc/a \tag{2.81}$$

  it is possible to recast the terms formally written as $\overline{\rho\phi\psi}$ in the following way

$$\overline{\rho\phi\psi} = \bar{\rho}\widetilde{\phi\psi} = \bar{\rho}\tilde{\phi}\tilde{\psi} + [G\star, H](\rho, \rho\phi, \rho\psi). \tag{2.82}$$

  For compressible flows, the subgrid scale (SGS) stress tensor results as

$$\tau_{ij} = [G\star, H](\rho, \rho u_i, \rho u_j) = \bar{\rho}(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j). \tag{2.83}$$

One should notice that this decomposition is not applied to the pressure and density fields. The filtered equation of state can then be written as

$$\bar{p} = \bar{\rho}R\tilde{T} \tag{2.84}$$

Quantities depending only on the temperature such as the enthalpy or the internal energy can also be Favre-filtered.

Theoretically, the use of this change of variable has important consequences concerning interpretation of results. HaMinh and Vandromme [107] remark that density weighted variables are well adapted to the comparison with experimental measurements carried out with hot wire anenometry. Conversely, they are less suitable for a comparison with data obtained by Laser Doppler Anenometry[5] for which the classical filtering operator is appropriate. Smits and Dussauge [266] evaluate the difference between mean velocity profiles of $\tilde{u}$ and $\bar{u}$ to about 1.5% in a $Ma = 3$ turbulent boundary layer. The comparison of LES results with DNS data must also be done with care, and, for proper comparisons DNS data should also be Favre-filtered.

2.3.7 Summary of the Different Type of Filters

As a summary, 3 different classes of filters have been identified in LES.

- The analytical filter represented by a convolution product is used for expressing the filtered Navier–Stokes equations.
- The filter associated to the computational grid. No frequency higher than the Nyquist frequency associated to this grid can be represented in the simulation.
- The filter induced by the numerical scheme. The error committed by approximating the partial derivative operators by discrete operators modifies the computed solution. This kind of error can be computed using the modified wave number formalism [283].

Additionally, it is possible to associate a filter to the model used to approximate the subgrid scale tensor.

The computed solution is the result of these filtering processes constituting the effective filter. When performing a computation the question arises as to what the effective filter is, that governs the dynamics of the numerical solution.

2.4 Formulation of the Filtered Governing Equations

In this section the different ways of filtering the momentum and energy equations are reviewed. Non conservative and conservative forms are presented. Due to the use of the aforementioned “Favre filtering”, the continuity equation becomes

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0. \tag{2.85}$$

In the particular case of an energy equation based on the total energy, the filtered momentum equation depends on the choice of the filtered pressure which may be different from the quantity obtained by applying a filter to the pressure.

[5] The same is also true for Particule Image Velocimetry.

2.4.1 Enthalpy Formulation

The enthalpy formulation is

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{h}\tilde{u}_j}{\partial x_j} - \frac{\partial \bar{p}}{\partial t} - \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \check{q}_j}{\partial x_j} - \check{\Phi}$$
$$= - \left[\frac{\partial \bar{\rho} C_p (\widetilde{T u_j} - \tilde{T}\tilde{u}_j)}{\partial x_j} - \left(\overline{u_j \frac{\partial p}{\partial x_j}} - \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} \right) - (\bar{\Phi} - \check{\Phi}) + \frac{\partial (\overline{q_j} - \check{q}_j)}{\partial x_j} \right] \tag{2.86}$$

where the filtered enthalpy $\tilde{h}$ is equal to $C_p\tilde{T}$ and the filtered computable viscous dissipation $\check{\Phi}$ is defined as

$$\check{\Phi} = \check{\sigma}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j}. \tag{2.87}$$

where

$$\check{\sigma}_{ij} = \mu(\tilde{T}) \left(2\tilde{S}_{ij} - \frac{2}{3}\delta_{ij}\tilde{S}_{kk} \right) \tag{2.88}$$

which depends on the computable rate-of-strain tensor

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \tag{2.89}$$

The computable heat flux is

$$\check{q}_j = -\kappa(\tilde{T}) \frac{\partial \tilde{T}}{\partial x_j}. \tag{2.90}$$

The non linearity introduced by Sutherland's law to viscosity and conductivity gives rise to the additional term $\overline{q_j} - \check{q}_j$ in the energy equation.

Using the following decomposition of the filtered pressure-gradient velocity correlation

$$\overline{u_j \frac{\partial p}{\partial x_j}} = \frac{\partial \overline{p u_j}}{\partial x_j} - \overline{p \frac{\partial u_j}{\partial x_j}} \tag{2.91}$$

$$= \frac{\partial \overline{\rho R T u_j}}{\partial x_j} - \overline{p \frac{\partial u_j}{\partial x_j}} \tag{2.92}$$

$$= \frac{\partial \bar{\rho} R \tilde{T} \tilde{u}_j}{\partial x_j} + \frac{\partial \bar{\rho} R (\widetilde{T u_j} - \tilde{T}\tilde{u}_j)}{\partial x_j} - \overline{p \frac{\partial u_j}{\partial x_j}} \tag{2.93}$$

$$= \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \bar{\rho} R (\widetilde{T u_j} - \tilde{T}\tilde{u}_j)}{\partial x_j} - \overline{p \frac{\partial u_j}{\partial x_j}} \tag{2.94}$$

in (2.86) leads to the following form for the enthalpy equation

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{h}\tilde{u}_j}{\partial x_j} - \frac{\partial \bar{p}}{\partial t} - \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \check{q}_j}{\partial x_j} - \check{\Phi}$$
$$= -\left[\frac{\partial C_v Q_j}{\partial x_j} + \Pi_{dil} - \epsilon_v + \frac{\partial(\overline{q_j} - \check{q}_j)}{\partial x_j} \right]. \tag{2.95}$$

The SGS temperature flux is defined as

$$Q_j = \bar{\rho}(\widetilde{u_j T} - \tilde{u}_j \tilde{T}). \tag{2.96}$$

The SGS pressure-dilatation can be written as

$$\Pi_{dil} = \overline{p\frac{\partial u_j}{\partial x_j}} - \bar{p}\frac{\partial \tilde{u}_j}{\partial x_j}. \tag{2.97}$$

The SGS viscous dissipation is expressed as

$$\epsilon_v = \bar{\Phi} - \check{\Phi}. \tag{2.98}$$

2.4.2 Temperature Formulation

Applying the filtering operation to (2.13) gives

$$\frac{\partial \bar{\rho} C_v \tilde{T}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j C_v \tilde{T}}{\partial x_j} + \bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} - \check{\Phi} + \frac{\partial \check{q}_j}{\partial x_j}$$
$$= -\left[\frac{\partial \overline{\rho u_j C_v T}}{\partial x_j} - \frac{\partial \bar{\rho}\tilde{u}_j C_v \tilde{T}}{\partial x_j} + \overline{p\frac{\partial u_j}{\partial x_j}} - \bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} - (\bar{\Phi} - \check{\Phi}) + \frac{\partial(\overline{q_j} - \check{q}_j)}{\partial x_j} \right], \tag{2.99}$$

which can be recast as

$$\frac{\partial \bar{\rho} C_v \tilde{T}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j C_v \tilde{T}}{\partial x_j} + \bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} - \check{\Phi} + \frac{\partial \check{q}_j}{\partial x_j}$$
$$= -\left[\frac{\partial C_v Q_j}{\partial x_j} + \Pi_{dil} - \epsilon_v + \frac{\partial(\overline{q_j} - \check{q}_j)}{\partial x_j} \right]. \tag{2.100}$$

The temperature formulation has been used with additional simplifications by Moin et al. [201]. It can also be found in its internal energy form in Ref. [192] by replacing $C_v\tilde{T}$ by $\tilde{\epsilon}$ in the first two terms.

2.4.3 Pressure Formulation

Applying the filtering operator to (2.14) gives

$$\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \gamma \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} - (\gamma - 1)\check{\Phi} + (\gamma - 1)\frac{\partial \check{q}_j}{\partial x_j}$$
$$= -\left[\overline{u_j \frac{\partial p}{\partial x_j}} - \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \gamma \overline{p \frac{\partial u_j}{\partial x_j}} - \gamma \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} - (\gamma - 1)(\bar{\Phi} - \check{\Phi}) \right.$$
$$\left. + (\gamma - 1) \frac{\partial (\overline{q_j} - \check{q}_j)}{\partial x_j} \right]. \tag{2.101}$$

Using the following decomposition:

$$u_j \frac{\partial p}{\partial x_j} + \gamma p \frac{\partial u_j}{\partial x_j} = u_j \frac{\partial p}{\partial x_j} + \gamma \left(\frac{\partial p u_j}{\partial x_j} - u_j \frac{\partial p}{\partial x_j} \right) \tag{2.102}$$
$$= \gamma \frac{\partial p u_j}{\partial x_j} - (\gamma - 1) u_j \frac{\partial p}{\partial x_j} \tag{2.103}$$

which can be employed both globally filtered or only with computable variables, the filtered pressure equation can be written as

$$\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \gamma \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} - (\gamma - 1)\check{\Phi} + (\gamma - 1)\frac{\partial \check{q}_j}{\partial x_j}$$
$$= -\left[\gamma R \frac{\partial Q_j}{\partial x_j} - (\gamma - 1)\left(\overline{u_j \frac{\partial p}{\partial x_j}} - \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} \right) - (\gamma - 1)(\bar{\Phi} - \check{\Phi}) \right.$$
$$\left. + (\gamma - 1) \frac{\partial (\overline{q_j} - \check{q}_j)}{\partial x_j} \right]. \tag{2.104}$$

It is possible to introduce a stronger separation between computable terms and terms to be modeled using (2.94). In this case (2.101) becomes

$$\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + \gamma \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} - (\gamma - 1)\check{\Phi} + (\gamma - 1)\frac{\partial \check{q}_j}{\partial x_j}$$
$$= -R \frac{\partial Q_j}{\partial x_j} - (\gamma - 1) \left[\Pi_{dil} - \epsilon_v + \frac{\partial (\overline{q_j} - \check{q}_j)}{\partial x_j} \right]. \tag{2.105}$$

2.4.4 Entropy Formulation

An equation for the Favre-filtered entropy can be written as

$$\frac{\partial \bar{\rho} \tilde{s}}{\partial t} + \frac{\partial \bar{\rho} \tilde{s} \tilde{u}_j}{\partial x_j} - \frac{1}{\tilde{T}} \left[\check{\Phi} + \frac{\partial}{\partial x_j} \left(\kappa(\tilde{T}) \frac{\partial \tilde{T}}{\partial x_j} \right) \right]$$
$$= -\frac{\partial \bar{\rho} (\widetilde{s u_j} - \tilde{s} \tilde{u}_j)}{\partial x_j} + \left(\overline{\frac{\Phi}{T}} - \frac{\check{\Phi}}{\tilde{T}} \right) + \overline{\frac{1}{T} \frac{\partial}{\partial x_j} \left(\kappa(T) \frac{\partial T}{\partial x_j} \right)}$$
$$- \frac{1}{\tilde{T}} \frac{\partial}{\partial x_j} \left(\kappa(\tilde{T}) \frac{\partial \tilde{T}}{\partial x_j} \right), \tag{2.106}$$

with $\tilde{s} = \frac{1}{\bar{\rho}} \overline{\rho C_v \ln(p \rho^{-\gamma})}$. Nevertheless, $\tilde{s}$ can not be easily linked to the computable entropy $\check{s} = C_v \ln(\bar{p} \bar{\rho}^{-\gamma})$. This reason may explain the fact that the equation for the filtered entropy has not yet been used in the literature in a form similar to (2.106). However, Mathew et al. [194] have used the entropy formulation in the ADM framework (see Chap. 5) which does not require any explicit modeling of the subgrid terms in the right hand side of (2.106).

2.4.5 Filtered Total Energy Equations

Applying the filtering operator to the total energy definition (2.4) leads to the following equation

$$\bar{\rho}\tilde{E} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2}\bar{\rho}\widetilde{u_i u_i} \tag{2.107}$$

which is not directly computable. This issue has been addressed in the literature using different techniques:

- Ragab and Sreedhar [226], Piomelli [216], Kosovic et al. [147], and Dubois et al. in a simplified form [61] write an equation of evolution for

$$\bar{\rho}\tilde{E} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i + \frac{\tau_{ii}}{2} \tag{2.108}$$

  which implies that the pressure and the temperature are computed as

$$\bar{p} = (\gamma - 1)\left[\bar{\rho}\tilde{E} - \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i - \frac{\tau_{ii}}{2}\right] \tag{2.109}$$

  and

$$\tilde{T} = \frac{(\gamma - 1)}{R}\left[\tilde{E} - \frac{1}{2}\tilde{u}_i\tilde{u}_i - \frac{\tau_{ii}}{2\bar{\rho}}\right], \tag{2.110}$$

  respectively. The equation of state is not affected.
- Vreman in its "system II" [306] introduces a change of variable on the pressure

$$\breve{P} = \bar{p} + \frac{(\gamma - 1)}{2}\tau_{ii} \tag{2.111}$$

  by which the trace of the SGS tensor in the energy equation disappears

$$\bar{\rho}\tilde{E} = \frac{\breve{P}}{(\gamma - 1)} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i. \tag{2.112}$$

  The temperature is also modified as

$$\breve{T} = \tilde{T} + \frac{\tau_{ii}}{2C_v\bar{\rho}}, \tag{2.113}$$

  leaving the equation of state formally unchanged

$$\breve{P} = \bar{\rho}R\breve{T}. \tag{2.114}$$

- Comte and Lesieur [47, 174] have proposed a different change of variable on the pressure which results in the so-called macro-pressure

$$\bar{\mathcal{P}} = \bar{p} + \frac{1}{3}\tau_{ii}. \tag{2.115}$$

This change of variable is motivated by an analogy with incompressible flows where the isotropic part of the SGS tensor is added to the pressure. The temperature is modified according to (2.113) so that the SGS stress tensor does not appear in the definition of the filtered energy equation if computed with $\breve{T}$. The equation of state takes the form

$$\bar{\mathcal{P}} = \bar{\rho} R \breve{T} - \frac{3\gamma - 5}{6}\tau_{ii}. \tag{2.116}$$

For a monoatomic gas such as argon or helium (for which $\gamma = 5/3$) equation (2.116) recovers the classical form.
- Vreman in its "system I" establishes an equation for the computable energy $\breve{E}$

$$\breve{E} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i. \tag{2.117}$$

This system does not require any modification of the thermodynamic variables.

A System for $\tilde{E}$, $\bar{p}$, $\tilde{T}$

The system can be written as

$$\begin{aligned} &\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{E} + \bar{p})\tilde{u}_j}{\partial x_j} - \frac{\partial \breve{\sigma}_{ij}\tilde{u}_i}{\partial x_j} + \frac{\partial \breve{q}_j}{\partial x_j} \\ &\quad = -\frac{\partial}{\partial x_j}[(\overline{\rho u_j E} - \bar{\rho}\tilde{u}_j\tilde{E}) + (\overline{u_j p} - \tilde{u}_j\bar{p}) - (\overline{\sigma_{ij}u_j} - \breve{\sigma}_{ij}\tilde{u}_j) - (\overline{q_j} - \breve{q}_j)]. \end{aligned} \tag{2.118}$$

It is possible to regroup the first two SGS terms of the right hand side of (2.118) in the following form

$$(\overline{\rho u_j E} - \bar{\rho}\tilde{u}_j\tilde{E}) + (\overline{u_j p} - \tilde{u}_j\bar{p}) = C_p Q_j + \mathcal{J}_j, \tag{2.119}$$

where

$$\mathcal{J}_j = \frac{1}{2}(\bar{\rho}\widetilde{u_j u_i u_i} - \bar{\rho}\tilde{u}_j\widetilde{u_i u_i}) = \frac{1}{2}(\bar{\rho}\widetilde{u_j u_i u_i} - \bar{\rho}\tilde{u}_j\tilde{u}_i\tilde{u}_i - \tau_{ii}) \tag{2.120}$$

is the SGS turbulent diffusion.

Introducing the SGS viscous diffusion

$$\mathcal{D}_j = \overline{\sigma_{ij}u_j} - \breve{\sigma}_{ij}\tilde{u}_j, \tag{2.121}$$

(2.118) can be rewritten as

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{E} + \bar{p})\tilde{u}_j}{\partial x_j} - \frac{\partial \breve{\sigma}_{ij}\tilde{u}_i}{\partial x_j} + \frac{\partial \breve{q}_j}{\partial x_j}$$
$$= -\frac{\partial}{\partial x_j}[C_p Q_j + \mathcal{J}_j - \mathcal{D}_j - (\overline{q_j} - \breve{q}_j)]. \qquad (2.122)$$

A System for $\tilde{E}$, $\breve{p}$, $\breve{T}$

With the aforementioned change of variable on pressure and temperature, Vreman, in its system II, writes the energy equation as

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{E} + \breve{p})\tilde{u}_j}{\partial x_j} - \frac{\partial \breve{\sigma}_{ij}\tilde{u}_i}{\partial x_j} + \frac{\partial \breve{q}_j}{\partial x_j} = -\frac{\partial}{\partial x_j}(C_p Q_j + \mathcal{J}_j - D_3 - D_4 + D_5), \qquad (2.123)$$

with

$$\breve{q}_j = -\kappa(\breve{T})\frac{\partial \breve{T}}{\partial x_j}. \qquad (2.124)$$

The term

$$D_3 = \frac{\partial}{\partial x_j}\left(\frac{\gamma - 1}{2}\tau_{ii}\tilde{u}_j\right) \qquad (2.125)$$

results from the difference between $\bar{p}$ and $\breve{p}$.

The difference between

$$D_4 = \frac{\partial}{\partial x_j}(\overline{\sigma_{ij}u_i} - \breve{\sigma}_{ij}\tilde{u}_i) \qquad (2.126)$$

and

$$D_5 = \frac{\partial}{\partial x_j}(\overline{q_j} - \breve{q}_j) \qquad (2.127)$$

and their counterparts in (2.122) arise from the (inexact) replacement of $\tilde{T}$ by $\breve{T}$ in the computable heat flux ($\breve{q}_j$)) and strain of rate tensor $\breve{\sigma}_{ij}$ which introduces additional terms involving τ_{ii}.

A System for $\tilde{E}$, $\bar{\mathcal{P}}$, $\breve{T}$

With this set of variables Comte and Lesieur [47] derive the following energy equation

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{E} + \bar{\mathcal{P}})\tilde{u}_j}{\partial x_j} - \frac{\partial \breve{\sigma}_{ij}\tilde{u}_i}{\partial x_j} + \frac{\partial \breve{q}_j}{\partial x_j} = -\frac{\partial}{\partial x_j}(\mathcal{Q}_j - D_4 + D_5) \qquad (2.128)$$

with

$$\mathcal{Q}_j = \overline{(\rho E + p)u_j} - (\bar{\rho}\tilde{E} + \bar{\mathcal{P}})\tilde{u}_j, \qquad (2.129)$$

which can be recast in a form similar to (2.119)

$$\mathcal{Q}_j = C_p Q_j + \mathcal{J}_j - \frac{1}{3}\tilde{u}_j\tau_{ii}. \qquad (2.130)$$

A System for $\check{E}$, $\bar{p}$, $\tilde{T}$

Vreman establishes the equation for the computable total energy adding the filtered internal energy equation to the filtered kinetic energy equation

$$\frac{\partial \check{E}}{\partial t}+\frac{\partial(\check{E}+\bar{p})\tilde{u}_j}{\partial x_j}-\frac{\partial \check{\sigma}_{ij}\tilde{u}_i}{\partial x_j}+\frac{\partial \check{q}_j}{\partial x_j}=-B_1-B_2-B_3+B_4+B_5+B_6-B_7. \quad (2.131)$$

The SGS terms B_i can be written as

$$B_1=\frac{1}{\gamma-1}\frac{\partial}{\partial x_j}(\overline{pu_j}-\bar{p}\tilde{u}_j)=\frac{\partial C_v Q_j}{\partial x_j}, \quad (2.132)$$

$$B_2=\overline{p\frac{\partial u_k}{\partial x_k}}-\bar{p}\frac{\partial \tilde{u}_k}{\partial x_k}=\Pi_{dil}, \quad (2.133)$$

$$B_3=\frac{\partial}{\partial x_j}(\tau_{kj}\tilde{u}_k), \quad (2.134)$$

$$B_4=\tau_{kj}\frac{\partial}{\partial x_j}\tilde{u}_k, \quad (2.135)$$

$$B_5=\overline{\sigma_{kj}\frac{\partial}{\partial x_j}u_k}-\overline{\sigma_{kj}}\frac{\partial}{\partial x_j}\tilde{u}_k=\epsilon_v, \quad (2.136)$$

$$B_6=\frac{\partial}{\partial x_j}(\overline{\sigma_{ij}}\widetilde{u}_i-\check{\sigma}_{ij}\widetilde{u}_i)=\frac{\partial \mathcal{D}_j}{\partial x_j}, \quad (2.137)$$

$$B_7=\frac{\partial}{\partial x_j}(\overline{q_j}-\check{q}_j). \quad (2.138)$$

The terms B_3 and B_4 are regrouped in the original work of Vreman [307]. The terms B_4 and B_5 can not be written in a conservative form. This might have some consequences for the treatment of flows with discontinuities.

2.4.6 Momentum Equations

In the vast majority of the published results, the selected system of equation is based on the filtered pressure $\bar{p}$. The filtered momentum equation is

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j}+\frac{\partial \bar{p}}{\partial x_i}-\frac{\partial \check{\sigma}_{ij}}{\partial x_j}=-\frac{\partial \tau_{ij}}{\partial x_j}+\frac{\partial}{\partial x_j}(\overline{\sigma_{ij}}-\check{\sigma}_{ij}). \quad (2.139)$$

In the particular case of the change of variables introduced by Vreman [306] in its system II, replacing $\bar{p}$ by $\check{P}$ in (2.139), an additional term $\frac{(\gamma-1)}{2}\tau_{ii}$ occurs on the right hand side of (2.139).
Using the change of variable proposed by Comte and Lesieur [47], $\mathcal{P}$ substitutes $\bar{p}$, and $\tau_{ii}/3$ is subtracted from the right hand side of (2.139). It is equivalent to a replacement of τ_{ij} by its deviatoric part τ_{ij}^d defined as

$$\tau_{ij}^d=\tau_{ij}-\delta_{ij}\tau_{kk}/3. \quad (2.140)$$

For the sake of completeness, one has to mention that in the case of the Vreman's system I $\check{\sigma}_{ij}$ should be replaced by $\check{\sigma}_{ij}$ in (2.139).

2.4.7 Simplifying Assumptions

SGS Force Terms

The different forms of the energy equation involve a large number of subgrid terms. Unfortunately, there are only two studies in which the forces of all subgrid terms have been computed using *a priori* tests.[6] The first one by Vreman et al. [306] and Vreman [307] is based on a 2D temporal shear layer. The convective Mach number effect has been investigated in the range 0.2–1.2. The 2D character of these simulations may limit the relevance of the conclusions drawn from this study. The other one is due to Martin et al. [192] who have carried out DNS of freely decaying homogeneous isotropic turbulence at a turbulent Mach number equal to 0.52.

In their study, Vreman et al. have compared the amplitude of the terms associated to resolved and SGS fields for their formulations I and II. Their conclusions are summarized in Table 2.3. The classification (large, medium, small, negligible) is based on the L_2 norm of the different terms of the filtered equations. One order of magnitude separates the norm of each class of terms. One can then expect that this classification may not hold locally.

Table 2.3. Classification of terms in the filtered energy equations

Influence of the term	System I	System II
Large	convective $\overline{NS}$	convective $\overline{NS}$
Medium	diffusive $\overline{NS}$, A_1, B_1, $B_2 = \Pi_{dil}$, B_3	diffusive $\overline{NS}$, C_1, D_1, D_2
Small	B_4, $B_5 = \epsilon_v$	D_3, D_4, D_5
Negligible	$\frac{\partial}{\partial x_j}(\overline{\sigma_{ij}} - \check{\sigma}_{ij})$, B_6, B_7	$\frac{\partial}{\partial x_j}(\overline{\sigma_{ij}} - \check{\sigma}_{ij})$

Martin et al. [192] have compared the main SGS terms appearing in the internal energy (2.100) and enthalpy (2.95) equations on the one hand and in the total energy equation (2.122) on the other hand. In the former cases they concluded that Π_{dil} is negligible, ϵ_v is one order of magnitude smaller than the divergence of the SGS heat flux ($C_v Q_j$). In the total energy equation (2.122), the SGS turbulent diffusion is comparable with the divergence of the SGS heat flux ($C_p Q_j$), and the SGS viscous diffusion ($\mathcal{D}_j$) is one order of magnitude smaller than the other terms.

From these two studies one can conclude that the non-linear terms occurring in the viscous terms and in the heat fluxes are small or negligible, depending on the chosen system. In practice, they are neglected by every authors. Specifically, this is equivalent to assume that $\overline{\sigma_{ij}} = \check{\sigma}_{ij}$ and $\overline{\sigma_{ij} u_i} = \check{\sigma}_{ij}\tilde{u}_i$. These two studies disagree on the importance of the $B_2 = \Pi_{dil}$ term. However, the respective conclusions are obtained for two different configurations

[6] Each term is computed on a DNS field and filtered on a LES grid. The forces of all terms are then compared.

and for two different systems of equations. In practice, this disagreement appears to have no significance. Martin et al. neglect this term and we will see in Chap. 4 that Vreman et al. model it together with B_1 so that eventually there is no model specific to this term published in the literature.

Small Scales Incompressibility

In order to present the different approaches developed in the literature, it is necessary to introduce the triple decomposition (adapted for compressible flows). A product of filtered terms can be decomposed

$$\overline{\rho\phi\psi} = \overline{\rho(\tilde{\phi} + \phi'')(\tilde{\psi} + \psi'')} \tag{2.141}$$

which can be recast as

$$\bar{\rho}\widetilde{\phi\psi} = \bar{\rho}(\widetilde{\tilde{\phi}\tilde{\psi}} + \widetilde{\tilde{\phi}\psi''} + \widetilde{\tilde{\psi}\phi''} + \widetilde{\phi''\psi''}). \tag{2.142}$$

A subgrid term can be expressed using the triple decomposition

$$\bar{\rho}(\widetilde{\phi\psi} - \tilde{\phi}\tilde{\psi}) = \mathbf{L} + \mathbf{C} + \mathbf{R}, \tag{2.143}$$

where one can distinguish:

- The Leonard term which relates only filtered quantities

$$\mathbf{L} = \bar{\rho}(\widetilde{\tilde{\phi}\tilde{\psi}} - \tilde{\phi}\tilde{\psi}). \tag{2.144}$$

- A cross term which represents the interactions between resolved scales and subgrid scales

$$\mathbf{C} = \bar{\rho}(\widetilde{\tilde{\phi}\psi''} + \widetilde{\tilde{\psi}\phi''}) \tag{2.145}$$

- A Reynolds term which accounts for interactions between subgrid scales

$$\mathbf{R} = \bar{\rho}(\widetilde{\phi''\psi''}). \tag{2.146}$$

The last two terms require modeling.

Restricting now the analysis to the subgrid scale tensor τ_{ij} ($\phi = u_i$ and $\psi = u_j$) and decomposing R_{ij} into an isotropic part R^i_{ij} and a deviatoric part R^d_{ij}, Erlebacher et al. [75] show that

$$R^i_{ij} = -\frac{1}{3}\gamma M^2_{sgs}\bar{p}\delta_{ij}, \tag{2.147}$$

where the subgrid Mach number M_{sgs} is defined as $M_{sgs} = \sqrt{q^2_{sgs}/\gamma R\tilde{T}}$ with $q^2_{sgs} = R_{ii}/\bar{\rho}$. Using DNS of isotropic turbulence these authors have found that the thermodynamic pressure is by far more important than R^i_{ij} for subgrid Mach numbers less than 0.4. The subgrid Mach number being lower than the turbulent Mach number, they also find that it is possible to neglect R^i_{ij} up to turbulent Mach numbers M_t as large as 0.6. This condition is valid for most of supersonic flows.

This subgrid-scales incompressibility hypothesis has been widely used. It has been extended from R^i_{ij} to τ^i_{ij} by many authors [47, 307, 226]. The main argument is that most of the compressibility effects are assumed to affect essentially the large scales. They are accounted for by resolved quantities. In this respect, it is much less restrictive to neglect the compressibility effect on sugbrid scales quantities than on quantities representing the whole turbulence spectrum (as in RANS) since subgrid scales fluctuations contain only a small part (typically a tenth of percent) of the fluctuating energy. One can anticipate that the limit usually taken equal to $M_t = 0.2$ [167] by which the compressibility effect must by taken into account in RANS simulations is not relevant in the framework of LES.

If the isotropic part of the SGS tensor is neglected, $\bar{\mathcal{P}}$ and $\check{P}$ degenerates towards $\bar{p}$, and $\check{T}$ degenerates towards $\tilde{T}$. Additionally, D_3 cancels out and $\mathcal{Q}_j$ can be identified as $C_p Q_j + \mathcal{J}_j$. Consequently, the systems based on $(\tilde{E}, \bar{p}, \tilde{T})$, $(\tilde{E}, \bar{\mathcal{P}}, \check{T})$, $(\tilde{E}, \check{P}, \check{T})$ become identical. The system based on $(\check{E}, \bar{p}, \tilde{T})$ preserves its character, and Vreman et al. use the Table 2.3 to argue that the latter system can be preferred since the contributions coming from the non-linearity in the viscous stresses and the heat fluxes are more important in the formulation II (D_4 and D_5) than in the formulation I (B_6 and B_7). Nevertheless, as already mentioned, these terms being both weak in intensity and difficult to model, they are commonly neglected in practical simulations. For the rest of this textbook, we will assume that this approximation holds. Furthermore, one has to notice that non conservative terms are present in system II. For B_1 and B_2 this is not an issue since we will see in Sect. 4.4 that this terms will be modeled with a conservative approximation. But once a model for τ_{ij} is chosen, B_4 can be computed explicitly and its non-conservative character remains. This consideration has motivated some authors to neglect also B_4. This in agreement with Vreman recommendation of modeling at least terms of "medium" importance (of the same order that the Navier-Stokes diffusive fluxes). According to Table 2.3, this remark concerns B_1, B_2 and B_3. This latter term is in conservative form and its modeling is not an issue since it results directly from the choice of τ_{ij}.

Comte and Lesieur justify their approach noticing that it is less restrictive to assume that the term $\frac{3\gamma-5}{6}\tau_{ii}$ is negligible in the state equation (2.116) than to assume that τ_{ii} is negligible. This statement has been motivated by the fact they used a global model for $\mathcal{Q}_j$ without making the decomposition (2.130), which depends explicitly on τ_{ii} [47].

2.5 Additional Relations for LES of Compressible Flows

This section is devoted to some additional relations which can result in further constraints on subgrid models.

2.5.1 Preservation of Original Symmetries

Governing equations of compressible flow dynamics have one-parameter symmetries which constitute a Lie group. Since LES is assumed to converge continuously towards DNS as the scale separation length vanishes, it is reasonable to require that LES governing equations should have the same symmetries as the unfiltered Navier–Stokes equations.[7] This will lead to a twofold constraint, since both the scale separation operator and subgrid models should be designed to preserve symmetries. Such a constraint has been devised in the incompressible case in a few articles (see Ref. [244] for a comprehensive review), the main conclusion being that symmetry-preserving scale separation operators are rare and that most existing subgrid models for incompressible flows violate at least one of the fundamental symmetries of the incompressible Navier–Stokes equations.

Such an analysis so far has not been performed for compressible LES. The scope of the present section is not to provide an extensive analysis, but to state the symmetries of compressible Navier–Stokes equations,[8] each symmetry being an additional constraint for the design of compressible LES models and theoretical filters. Let us also note that, numerical methods should also preserve symmetries of the continuous equations. This point, however will not be further discussed here, but let us mention the fact that many numerical schemes violate very fundamental symmetries such as Galilean invariance.

We restrict ourself to the case of a perfect gas. The symmetries are summarized in Table 2.4. The different cases correspond to possible choices of physical variables with respect to the symmetry. In the most general case, viscosity (and therefore diffusivity) is considered as an autonomous variable. As simplification, it can be considered as a function of temperature (e.g. through the Sutherland law), or a constant parameter. The ultimate simplification consists in considering inviscid fluids, i.e. the symmetries of the Euler equations.

[7] Note that the use of statistical averaging operator may result in a change of the fundamental symmetries of a system, an illustrative example being the loss of time reversal symmetry in statistical thermodynamics: while individual molecule behavior may be time-reversed, the mean behavior of an ensemble of molecules obeys the second law of thermodynamics.

[8] The full set of one-parameter symmetries of compressible Navier–Stokes equations is unpublished to the knowledge of the authors. The full Lie group of symmetries displayed in this section was determined by D. Razafindralandy and A. Hamdouni [227], whose contribution is gratefully acknowledged.

Table 2.4. One-parameter Lie group of symmetries of compressible Navier–Stokes equations. In the Basic Case, time, space, velocity, pressure, density and molecular viscosity are assumed to vary independently. Diffusivity is tied to viscosity assuming that the Prandtl number is constant. This case can be simplified assuming that the viscosity is a temperature-dependent variable. The problem is further simplified assuming that $\mu = \kappa = 0$. The parameter of the transformation is denoted a in the scalar case and $\mathbf{a}$ is the vector case. $\mathbf{R}$ is a 3D time-independent rotation matrix

Symmetry name	Definition	Basic case	$\mu = \mu(T)$	Constant μ	$\mu = \kappa = 0$
Time shift	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t + a, \mathbf{x}, \mathbf{u}, p, \rho, \mu)$	yes	yes	yes	yes
Space shift	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t, \mathbf{x} + \mathbf{a}, \mathbf{u}, p, \rho, \mu)$	yes	yes	yes	yes
Galilean transform	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t, \mathbf{x} + \mathbf{a}t, \mathbf{u} + \mathbf{a}, p, \rho, \mu)$	yes	yes	yes	yes
3D rotation	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t, \mathbf{Rx}, \mathbf{Ru}, p, \rho, \mu)$	yes	yes	yes	yes
Scaling 1	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (e^{2a}t, e^{a}\mathbf{x}, e^{-a}\mathbf{u}, e^{-2a}p, \rho, \mu)$	yes	no	yes	yes
Scaling 2	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t, e^{a}\mathbf{x}, e^{a}\mathbf{u}, p, e^{-2a}\rho, \mu)$	yes	no	yes	yes
(Scaling 1) $\circ$ (Scaling 2)	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (e^{a}t, e^{a}\mathbf{x}, \mathbf{u}, p, e^{-a}\rho, \mu)$	yes	yes	yes	yes
Scaling 3	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu) \longrightarrow (t, \mathbf{x}, \mathbf{u}, e^{a}p, e^{a}\rho, e^{a}\mu)$	yes	no	no	no
Scaling 4	$(t, \mathbf{x}, \mathbf{u}, p, \rho, \mu = 0) \longrightarrow (t, \mathbf{x}, \mathbf{u}, e^{a}p, e^{a}\rho, \mu = 0)$	no	no	no	yes

2.5.2 Discontinuity Jump Relations for LES

Shock Modeling and Jump Relations

The present discussion will be restricted to the inviscid case for the sake of simplicity. The rationale for that is that viscous effects are negligible compared to other physical mechanisms during the interaction (as can be proved a posteriori by comparing theoretical results with DNS and experimental results), and that relaxation times associated to vibrational, rotational and translational energy modes of the molecules are very small with respect to macroscopic turbulent time scales. Therefore, the shock is modeled as a surface discontinuity with zero thickness. An important consequence is that the shock has no intrinsic time or length scale, and its corrugation is entirely governed by incident fluctuations. Its effects are entirely represented by the Rankine–Hugoniot jump conditions for the mass, momentum and energy:

$$[[\rho u_n]] = 0, \tag{2.148}$$

$$[[\rho u_n^2 + p]] = 0, \tag{2.149}$$

$$[[\boldsymbol{u}_t]] = 0, \tag{2.150}$$

$$\left[\left[e + \frac{p}{\rho} + u^2\right]\right] = [[H]] = 0, \tag{2.151}$$

where H is the stagnation enthalpy and $\boldsymbol{u}$ is the velocity in the reference frame of the shock wave, i.e. $\boldsymbol{u} = \boldsymbol{v} - \boldsymbol{u}_s$ where $\boldsymbol{v}$ and $\boldsymbol{u}_s$ are the fluid velocity and the shock speed in the laboratory frame, respectively. Subscripts n and t are related to the normal and tangential components of vector fields with respect to the shock wave, respectively

$$u_n \equiv \boldsymbol{u} \cdot \boldsymbol{n}, \qquad \boldsymbol{u}_t \equiv \boldsymbol{n} \times (\boldsymbol{u} \times \boldsymbol{n}), \qquad \boldsymbol{u} = u_n \boldsymbol{n} + \boldsymbol{u}_t, \tag{2.152}$$

where $\boldsymbol{n}$ is the shock normal unit vector.

An exact general jump condition for the vorticity can be derived from the relations given above [110]. First noting that the vorticity vector $\boldsymbol{\Omega} = \nabla \times \boldsymbol{u}$ can be decomposed as $\boldsymbol{\Omega} = \Omega_n \boldsymbol{n} + \boldsymbol{\Omega}_t$ with

$$\Omega_n = (\nabla \times \boldsymbol{u}_t)_n \tag{2.153}$$

and

$$\boldsymbol{\Omega}_t = \boldsymbol{n} \times \left(\frac{\partial \boldsymbol{u}_t}{\partial n} + \boldsymbol{u}_t \cdot \nabla \boldsymbol{n} - \nabla_{||} u_n \right) \tag{2.154}$$

where $\nabla_{||}$ denotes the tangential (with respect to the shock surface) part of the gradient operator, one obtains the following vorticity jump conditions in unsteady flows in which the shock experiences deformations

$$[[\Omega_n]] = 0, \tag{2.155}$$

$$[[\boldsymbol{\Omega}_t]] = \boldsymbol{n} \times \left(\nabla_{||}(\rho u_n) \left[\left[\frac{1}{\rho}\right]\right] - \frac{1}{\rho u_n}[[\rho]](D_{||}\boldsymbol{u}_t + u_s D_{||}\boldsymbol{n}) \right), \tag{2.156}$$

with

$$D_{||}\boldsymbol{u}_t = \left(\frac{d\boldsymbol{u}_t}{dt}\right)_t + \boldsymbol{u}_t \cdot \nabla_{||}\boldsymbol{u}_t = \left(\frac{\partial \boldsymbol{u}_t}{\partial t} + u_s \frac{\partial \boldsymbol{u}_t}{\partial n}\right)_t + \boldsymbol{u}_t \cdot \nabla_{||}\boldsymbol{u}_t \tag{2.157}$$

and

$$D_{||}\boldsymbol{n} = \frac{d\boldsymbol{n}}{dt} + \boldsymbol{u}_t \cdot \nabla_{||}\boldsymbol{n} = -\nabla_{||}u_s + \boldsymbol{u}_t \cdot \nabla_{||}\boldsymbol{n}. \tag{2.158}$$

It can be seen that the normal component of the vorticity is continuous across the shock, while the jump of the tangential component depends on the density jump, the tangential velocity and the shock wave deformation. In steady flows, the jump condition for the tangential vorticity simplifies as

$$[[\boldsymbol{\Omega}_t]] = \boldsymbol{n} \times \left(\nabla_{||}(\rho u_n) \left[\left[\frac{1}{\rho}\right]\right] - \frac{1}{\rho u_n}[[\rho]]\, \boldsymbol{u}_t \cdot \nabla_{||}\boldsymbol{u}_t \right). \tag{2.159}$$

Filtered Jump Relations and Associated Constrains on Subgrid Terms

The question of deriving pseudo-jump relation for coarse resolution simulations, such as LES, is not a trivial task since several fundamental issues arise.

First, one has to decide if the LES solution can exhibit discontinuities. If it is assumed that LES governing equations originate from the application of a smoothing (i.e. regularizing) kernel to the exact equations, discontinuities are transformed into regions with large gradients but finite thickness. Therefore, jump conditions no longer hold, and must be replaced by classical global conservation laws. Such global relations are obtained by performing a volume integration of the LES governing equations over a control cell that encompasses the initial discontinuity.

The second issue comes from the relation between the grid size and the scale separation length. In almost all published works, authors have considered these lengthscales to be equal or very close. As a consequence, the large gradient region cannot be accurately computed on the grid, due to numerical errors. Therefore, jump relations are explicitly or implicitly used in practice to design shock-capturing techniques which yield entropic solutions. Here, the coupling between numerical discretization and the continuous LES formalism is obvious. It is worth noting that in the case of reacting flows with flames, the *thickened flame* approach has been proposed (see e.g. [220]) to allow for an accurate description of the dynamics inside the flame front, but the approach is not fully consistent in the sense that the thickened flame and the filtered turbulent field are not be obtained using a unique filtering operator. Extension of this approach to general discontinuities remains to be done.

A third issue is that pseudo-jump relations introduce additional constraints on subgrid models, which are not taken into account in most subgrid model derivations. To illustrate this point, let us consider the simple case in which LES pseudo-jump relations are obtained in a straightforward manner by applying the scale separation operator to the exact jump relations (2.148)–(2.151). One obtains (different forms can be obtained selecting other sets of filtered variables)

$$[[\overline{\rho u_n}]] = [[\overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{n}}]] + \underbrace{[[\overline{\rho u_n} - \overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{n}}]]}_{\text{subgrid}} = 0, \tag{2.160}$$

$$[[\overline{\rho u_n^2} + \bar{p}]] = \left[\left[\frac{(\overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{n}})^2}{\bar{\rho}} + \bar{p}\right]\right] + \underbrace{\left[\left[\overline{\rho u_n^2} - \frac{(\overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{n}})^2}{\bar{\rho}}\right]\right]}_{\text{subgrid}} = 0, \tag{2.161}$$

$$[[\overline{\boldsymbol{u}_t}]] = [[\overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{t}}]] + \underbrace{[[\overline{\rho u_t} - \overline{\rho \boldsymbol{u}} \cdot \bar{\boldsymbol{t}}]]}_{\text{subgrid}} = 0, \tag{2.162}$$

$$\begin{aligned}\left[\left[\bar{e} + \overline{\left(\frac{p}{\rho}\right)} + \overline{u^2}\right]\right] &= \left[\left[\bar{e} + \left(\frac{\bar{p}}{\bar{\rho}}\right) + \bar{\boldsymbol{u}} \cdot \bar{\boldsymbol{u}}\right]\right] \\ &+ \underbrace{\left[\left[\left(\overline{\left(\frac{p}{\rho}\right)} - \left(\frac{\bar{p}}{\bar{\rho}}\right)\right) + (\overline{u^2} - \bar{\boldsymbol{u}} \cdot \bar{\boldsymbol{u}})\right]\right]}_{\text{subgrid}} = 0.\end{aligned} \tag{2.163}$$

It is observed that subgrid terms contribute to the jump relations which hold for the resolved scales. Therefore, the subgrid jump terms should ideally be taken into account to recover a fully satisfactory behavior of the computed solution in the vicinity of shock waves. It is worthy noting that subgrid jump terms differ from those found in the governing filtered equations.

2.5.3 Second Law of Thermodynamics

Compressible flow simulations raise the question of the compatibility of the computed solution with fundamental laws of thermodynamics. We now discuss the case of the second law of thermodynamics. It is worth noting that it is a non linear relation. Therefore, the filtered field does not a priori obey it, in the same way that it does not fulfill the original Navier–Stokes equations since nonlinearities give rise to subgrid residuals. As a consequence, the LES solution obeys new extended thermodynamic constraints, which are obtained by applying the scale-separation operator to the classical thermodynamic laws.

The Clausius-Duhem entropy inequality, using (2.15), can be recast as

$$\frac{1}{T}\left[\Phi + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\right] \geq 0. \tag{2.164}$$

Multiplying this relation by T and applying a *positive* scale-separation operator, one obtains

$$\bar{\Phi} + \overline{\frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)} \geq 0 \tag{2.165}$$

which appears as an exact extension of the second law of thermodynamics for LES. It can be further refined by including the resolved and subgrid contributions

$$\check{\Phi} + \epsilon_v + \frac{\partial \check{q}_j}{\partial x_j} + B_7 \geq 0. \tag{2.166}$$

This last equation shows that the subgrid viscous dissipation ϵ_v (defined in (2.98)) and the subgrid viscous heat flux B_7 (see (2.138)) cannot be computed independently, since they are bounded by the second law of thermodynamics. Subgrid models which satisfy (2.166) can be referred to as *thermodynamically consistent* subgrid models, by analogy with previous works carried out within the RANS framework [9, 237, 238].

2.6 Model Construction

In the previous sections, we have shown that the reduction of the solution complexity (number of degree of freedom) in space and time by the filtering process results in coupling terms between resolved scales and subfilter scales that must be closed by an appropriate form of modeling. The modeling process consists in approximating the coupling terms on the basis of the information contained solely in the resolved scales. Among all the SGS terms, τ_{ij} possesses a particular status since it is the only term which appears in the equations for an incompressible isothermal fluid. One can anticipate that it will also play an important role for compressible flows.

2.6.1 Basic Hypothesis

Subgrid modeling usually is based on the following hypothesis: *If subgrid scales exist, then the flow is locally (in space and time) turbulent.* Consequently, the subgrid models will be built on the known properties of turbulent flows that will be summarized in chapter 3. Before discussing the various ways of modeling the subgrid terms, we have to set some constraints [244]. The subgrid modeling must be done in compliance with two types of constraints:

- Physical constraints. The model must be consistent from the viewpoint of the phenomenon being modeled, i.e.:
  - Conserve the basic properties of the underlying equations, such as Galilean invariance and asymptotic behavior;
  - Vanish wherever the exact solution exhibits no small scales corresponding to the subgrid scales;
  - Induce an effect of the same kind (dispersive or dissipative, for example) as the modeled terms;
  - Not destroy the dynamics of the resolved scales, and thus especially not inhibit the flow driving mechanisms.

- Numerical constraints. A subgrid model can only be thought of as part of a numerical simulation method, and must consequently:
  - Be of acceptable algorithmic cost, and especially be local in time and space;
  - Not destabilize the numerical simulation;
  - Be insensitive to discretization, i.e. the physical effects induced theoretically by the model must not be inhibited by the discretization.

2.6.2 Modeling Strategies

The problem of subgrid modeling consists in taking the interaction with the fluctuating field ϕ' into account in the evolution equation of the filtered field $\bar{\phi}$. Two modeling strategies exist [244]:

- *Structural modeling* of the subgrid term, which consists in making the best approximation of the modeled terms by constructing from an evaluation of $\bar{\phi}$ or a formal series expansion.
- *Functional modeling*, which consists in modeling the action of the subgrid terms on the quantity $\bar{\phi}$ and not the modeled term itself, i.e. introducing a dissipative or dispersive term, for example, that has a similar effect but not necessarily the same structure.

The structural approach requires no knowledge of the nature of the scale interaction, but does require sufficient knowledge of the structure of the small scales, and one of the two following conditions has to be met:

- The dynamics of the equation being computed leads to a universal form of the small scales (and therefore to their structural independence from the resolved motion, as all that remains to be determined is their energy level).
- The dynamics of the equation induces a sufficiently strong and simple scale correlation for the structure of the subgrid scales to be deduced from the information contained in the resolved field. This require both a knowledge of the nature of the scale interaction and an universal character of the small scales.

The distinction between these two types of modeling is fundamental and structures the presentation of subgrid models in Chaps. 4 and 5.

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