23.2 Large Eddy Simulation

Large Eddy Simulation provides a compromise between DNS, where all scales of turbulence are computed directly from the Navier-Stokes equations, and RANS equations, where all scales of turbulence must be modeled. In Large Eddy Simulation, small-scale turbulence is filtered out from the Navier-Stokes equations, and a model is used to evaluate small scales. The resulting filtered Navier-Stokes equation is solved for the large-scale motion, which is responsible for most of momentum and energy transport. The large scale of motion is highly dependent on the flow conditions and geometries under consideration. The small scales are computed from the turbulence model known as the ***subgridscale model***, which in turn influence the large eddies. Since the small-scale eddies are more or less universal and homogeneous, it is postulated that the subgridscale model would be applicable to a wide range of flow regimes and conditions. Recall that the turbulence models for RANS are very much limited on the range of applications, because they attempt to model a wide range of scales and the random motion of eddies with no organized behavior.

In the following sections, descriptions of filtered Navier-Stokes equations for LES computations and typical subgrid models are presented.

23.2.1 Filtered Navier-Stokes Equations

In order to explore the concept of filtering, consider a simple example of central difference approximation expressed as

$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{\Delta x} = \frac{f(x+\Delta x/2) - f(x-\Delta x/2)}{\Delta x} \tag{23-1}$$

This expression simply approximates the derivative at point i as the averaged values of dependent variable at locations $i + \frac{1}{2}$ and $i - \frac{1}{2}$. Therefore, the expression (23-1) can be written as

$$\frac{1}{\Delta x}\left[f(x+\Delta x/2) - f(x-\Delta x/2)\right] = \frac{d}{dx}\left[\frac{1}{\Delta x}\int_{x-\Delta x/2}^{x+\Delta x/2} f(\xi)d\xi\right] \tag{23-2}$$

which may be interpreted as a filtering operator for which any scale smaller than Δx is filtered out. Now, a filtered quantity is defined as

$$\bar{f}_i(x) = \frac{1}{\Delta}\int_{x-\Delta/2}^{x+\Delta/2} f(\xi)d\xi = \int_{x-\Delta/2}^{x+\Delta/2} f(\xi)G(x,\xi)d\xi \tag{23-3}$$

where, in this case, $G(x,\xi) = 1/\Delta$, G is called a filter function, and Δ is the filter width. Typically, a filter over the entire domain is defined such that

$$\bar{f}(x) = \int_D f(\xi)G(x,\xi)d\xi \tag{23-4}$$

It can be shown that if G is a function of $(x - \xi)$, then differentiation and filtering operation commute [23.1]. Now, (23-4) is written as

$$\bar{f}(x) = \int_D f(\xi)G(x - \xi)d\xi \tag{23-5}$$

Some examples of one-dimensional filter functions are:

1. Top hat filter, $G(x - \xi) = \begin{cases} \dfrac{1}{\Delta} & \text{if } \mid x - \xi \mid < \Delta/2 \\ 0 & \text{otherwise} \end{cases}$

2. Gaussian filter, $G(x - \xi) = \left(\dfrac{6}{\pi\Delta^2}\right)^{3/2} \exp\left[- 6\dfrac{\mid x - \xi \mid^2}{\Delta^2}\right]$

The concept of filtering is extended to three dimensions by the following

$$\bar{f}(x_{i,t}) = \int_D f(\xi_i)G(x_i - \xi_i)d^3\xi_i \tag{23-6}$$

where $x_i = x, y, z$ and $\xi_i = \xi, \eta, \zeta$

Now, define any fluctuation at scales smaller than grid scale Δ as the subgrid scale (SGS) or unresolved quantity, and denote it by a prime. As defined previously by (23-4), the filtered or resolved quantity is denoted by an overbar. Thus,

$$f = \bar{f} + f' \tag{23-7}$$

With the definitions of the resolved and unresolved quantities completed, the Navier-Stokes equations are now modified to yield the Filtered Navier-Stokes (FNS) equations. The FNS equations govern the evolution of large-scale eddies. It will be given for an incompressible flow initially, and, subsequently it will be extended to compressible flows.

After the application of a filtering process, the incompressible Navier-Stokes equations become

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \tag{23-8}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i \bar{u}_j) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{23-9}$$

where τ_{ij} is the subgridscale stress term which represents the effect of small scales. The subgrid scale stress is given by

$$\tau_{ij} = \bar{u}_i\bar{u}_j - \overline{u_i u_j} \tag{23-10}$$

which, with the substitution of

$$\bar{u}_i = u_i - u_i' \tag{23-11}$$

can be written as

$$\begin{aligned} \tau_{ij} &= \bar{u}_i\bar{u}_j - \overline{\bar{u}_i\bar{u}_j} - \overline{\bar{u}_i u'_j} - \overline{u'_j\bar{u}_i} - \overline{u'_i u'_j} \\ &= L_{ij} + C_{ij} + R_{ij} \end{aligned} \qquad (23\text{-}12)$$

The terms L_{ij}, C_{ij}, and R_{ij} are defined as follows:

$L_{ij} = \bar{u}_i\bar{u}_j - \overline{\bar{u}_i\bar{u}_j}$ is called *Leonard stress,*

$C_{ij} = -(\overline{\bar{u}_i u'_j} - \overline{u'_j\bar{u}_i})$ is called *cross term stress,* and

$R_{ij} = -\overline{u'_i u'_j}$ is called the *subgridscale Reynolds stress*

Observe that the Leonard stress involves only the resolved quantities, and therefore it can be explicitly computed. Furthermore, note that this term represents the interaction of resolved scales which contribute and affect subgrid scales. The cross term stress and the SGS Reynolds stress involve unresolved quantities and must be modeled. The cross stress term represents the interaction of resolved and unresolved scales, whereas the SGS Reynolds stress represents the interaction of unresolved scales.

It is important to note that a filtered quantity represented by an overbar, that is, $\bar{f}$, is different from the averaging process used in the RANS equation, in particular $\bar{\bar{f}} \neq \bar{f}$.

It is common to rearrange Equation (23-9) and rewrite it as

$$\begin{aligned} \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i\bar{u}_j) &= -\frac{1}{\rho}\frac{\partial}{\partial x_i}\left(\bar{p} - \frac{1}{3}\rho\tau_{kk}\right)\delta_{ij} \\ &\quad + \nu\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}\right) \\ &= -\frac{1}{\rho}\frac{\partial p^+}{\partial x_j} + \nu\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + \frac{\partial \tau_{ij}^+}{\partial x_j} \end{aligned} \qquad (23\text{-}13)$$

where a modified pressure is defined as

$$p^+ = \bar{p} - \frac{1}{3}\rho\tau_{kk} \qquad (23\text{-}14)$$

and

$$\tau_{ij}^+ = \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} \qquad (23\text{-}15)$$

Extension of the FNS equations to compressible flow is straightforward except that Favre-filtering is used. As in the case of Favre- (or mass-) averaged Navier-Stokes equations, this approach is taken in order to prevent introduction of subgridscale terms into the continuity equation. A Favre-filtered quantity is defined as

$$\tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}} \tag{23-16}$$

Now, the Favre-filtered Navier-Stokes equations are written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = 0 \tag{23-17}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial \bar{p}}{\partial x_i} = \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{23-18}$$

As in the case of incompressible flow, Equation (23-18) is rearranged as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial \bar{p}}{\partial x_i}\delta_{ij} - \frac{1}{3}\frac{\partial \tau_{kk}}{\partial x_i}\delta_{ij} = \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{1}{3}\frac{\partial \tau_{kk}}{\partial x_j}\delta_{ij} \tag{23-19}$$

or

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial}{\partial x_i}\left(\bar{p} - \frac{1}{3}\tau_{kk}\right)\delta_{ij} = \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}\right) \tag{23-20}$$

Define a modified pressure p^+ as

$$p^+ = \bar{p} - \frac{1}{3}\tau_{kk} \tag{23-21}$$

and

$$\tau_{ij}^+ = \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} \tag{23-22}$$

Then, the momentum equation is written as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial p^+}{\partial x_j}\delta_{ij} = \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^+}{\partial x_j} \tag{23-23}$$

where

$$\tilde{\tau}_{ij} = -\frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) = \overline{\mu\, S_{ij}} \tag{23-24}$$

is the filtered stress term and

$$S_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \tag{23-25}$$

Furthermore,

$$\tau_{ij} = \bar{\rho}(\tilde{u}_i\tilde{u}_j - \widetilde{u_i u_j}) = \overline{\rho u_i}\,\overline{\rho u_j}/\bar{\rho} - \overline{\rho u_i u_j} \tag{23-26}$$

is the subgrid scale stress.

Note that at this point the subgridscale stress τ_{ij} appearing in Equation (23-20) is an additional unknown which must be modeled. Furthermore, the introduction of τ_{kk} in relations (23-21) and (23-22) and the question of how it may be computed need to be deliberated. These issues will be addressed shortly. For now, the goal is to establish the required set of filtered Navier-Stokes equations for LES of compressible flows. To complete the system of equations, consider the filtered energy equation expressed as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}_t) + \frac{\partial}{\partial x_i}\left[\overline{(\rho e_t + p)u_i}\right] = \frac{\partial}{\partial x_i}\left(\overline{k\frac{\partial T}{\partial x_i}}\right) + \frac{\partial}{\partial x_i}(\overline{\mu S_{ij}u_j}) \tag{23-27}$$

where

$$\bar{\rho}\tilde{e}_t = \bar{\rho}\tilde{e} + \frac{1}{2}\bar{\rho}(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2) - \frac{1}{2}\tau_{kk} \tag{23-28}$$

With the assumption of perfect gas, the total energy given by relation (23-28) can be written as

$$\bar{\rho}\tilde{e}_t = c_v\bar{\rho}\tilde{T} + \frac{1}{2}\bar{\rho}(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2) - \frac{1}{2}\tau_{kk} \tag{23-29}$$

which can be rearranged as

$$\bar{\rho}\tilde{e}_t = c_v\bar{\rho}\left(\tilde{T} - \frac{\tau_{kk}}{2c_v\bar{\rho}}\right) + \frac{1}{2}\bar{\rho}(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2) \tag{23-30}$$

Consistent with the definition of modified pressure, define a modified temperature as

$$T^+ = \tilde{T} - \frac{\tau_{kk}}{2c_v\bar{\rho}} \tag{23-31}$$

Subsequently

$$\bar{\rho}\tilde{e}_t = c_v\bar{\rho}T^+ + \frac{1}{2}\bar{\rho}(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2) \tag{23-32}$$

Consider also the equation of state for a perfect gas which, in terms of the filtered quantities, is written as

$$\bar{p} = \bar{\rho}R\tilde{T} \tag{23-33}$$

In order to write the equation of state given by (23-33) in terms of modified pressure and modified temperature, consider the following

$$\bar{p} - \frac{1}{3}\tau_{kk} = \bar{\rho}R\tilde{T} - \frac{1}{3}\tau_{kk} - \frac{\tau_{kk}}{2c_v\bar{\rho}}\bar{\rho}R + \frac{\tau_{kk}}{2c_v\bar{\rho}}\bar{\rho}R =$$

$$\bar{\rho}R\left(\tilde{T} - \frac{\tau_{kk}}{2c_v\bar{\rho}}\right) + \tau_{kk}\left(\frac{R}{2c_v} - \frac{1}{3}\right)$$

or

$$p^+ = \bar{\rho} R T^+ + \left(\frac{R}{2c_v} - \frac{1}{3} \right) \tau_{kk} \tag{23-34}$$

Now the energy equation given by (23-27) is written in terms of the modified pressure. Consider the second term given by $\overline{(\rho\, e_t + p) u_i}$ and rewrite it as

$$\begin{aligned} \overline{(\rho\, e_t + p) u_i} &= \overline{(\rho\, e_t + p) u_i} - (\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i + (\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i \\ &= -\, Q_i + (\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i \end{aligned} \tag{23-35}$$

where

$$Q_i = -\overline{(\rho\, e_t + p) u_i} + (\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i \tag{23-36}$$

is the subgrid heat flux. Thus, the energy equation is now written as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}_t) + \frac{\partial}{\partial x_i}\left[(\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i \right] = \frac{\partial Q_i}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\overline{k \frac{\partial T}{\partial x_i}} \right) + \frac{\partial}{\partial x_i}\left(\overline{\mu\, u_j\, S_{ij}} \right) \tag{23-37}$$

For a relatively high Reynolds number, typically the following is introduced in the momentum and energy equations, respectively.

$$\overline{\mu\, S_{ij}} = \mu\, \tilde{S}_{ij} \tag{23-38}$$

and

$$\overline{\mu\, u_j\, S_{ij}} = \mu\, \tilde{u}_j\, \tilde{S}_{ij} \tag{23-39}$$

Thus, the system of equations composed of filtered continuity, momentum, and energy equations is written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = 0 \tag{23-40}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j + p^+\delta_{ij}) = \frac{\partial \tau_{ij}^+}{\partial x_j} + \frac{\partial}{\partial x_j}(\mu\, \tilde{S}_{ij}) \tag{23-41}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}_t) + \frac{\partial}{\partial x_i}\left[(\bar{\rho}\tilde{e}_t + p^+)\tilde{u}_i \right] = \frac{\partial Q_i}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\overline{k \frac{\partial T}{\partial x_i}} \right) + \frac{\partial}{\partial x_i}(\mu\, \tilde{u}_j\, \tilde{S}_{ij}) \tag{23-42}$$

These equations are now expanded in Cartesian coordinate and are written in a flux vector formulation by defining

$$Q = \begin{bmatrix} \bar{\rho} \\ \bar{\rho}\tilde{u} \\ \bar{\rho}\tilde{v} \\ \bar{\rho}\tilde{w} \\ \bar{\rho}\tilde{e}_t \end{bmatrix} \tag{23-43}$$

$$E = \begin{bmatrix} \bar{\rho}\tilde{u} \\ \bar{\rho}\tilde{u}^2 + p^+ \\ \bar{\rho}\tilde{u}\tilde{v} \\ \bar{\rho}\tilde{u}\tilde{w} \\ (\bar{\rho}\tilde{e}_t + p^+)\tilde{u} \end{bmatrix} \tag{23-44}$$

$$F = \begin{bmatrix} \bar{\rho}\tilde{v} \\ \bar{\rho}\tilde{v}\tilde{u} \\ \bar{\rho}\tilde{v}^2 + p^+ \\ \bar{\rho}\tilde{v}\tilde{w} \\ (\bar{\rho}\tilde{e}_t + p^+)\tilde{v} \end{bmatrix} \quad (23\text{-}45) \qquad G = \begin{bmatrix} \bar{\rho}\tilde{w} \\ \bar{\rho}\tilde{w}\tilde{u} \\ \bar{\rho}\tilde{w}\tilde{v} \\ \bar{\rho}\tilde{w}^2 + p^+ \\ (\bar{\rho}\tilde{e}_t + p^+)\tilde{w} \end{bmatrix} \quad (23\text{-}46)$$

$$E_v = \begin{bmatrix} 0 \\ \tau^+_{xx} + \mu\,\tilde{S}_{xx} \\ \tau^+_{xy} + \mu\,\tilde{S}_{xy} \\ \tau^+_{xz} + \mu\,\tilde{S}_{xz} \\ Q_x + k\dfrac{\partial T^+}{\partial x} + \mu\,(\tilde{u}\tilde{S}_{xx} + \tilde{v}\,\tilde{S}_{xy} + \tilde{w}\,\tilde{S}_{xz}) \end{bmatrix} \quad (23\text{-}47)$$

$$F_v = \begin{bmatrix} 0 \\ \tau^+_{yx} + \mu\,\tilde{S}_{yx} \\ \tau^+_{yy} + \mu\tilde{S}_{yy} \\ \tau^+_{yz} + \mu\tilde{S}_{yz} \\ Q_y + k\dfrac{\partial T^+}{\partial y} + \mu\,(\tilde{u}\tilde{S}_{yx} + \tilde{v}\,\tilde{S}_{yy} + \tilde{w}\,\tilde{S}_{yz}) \end{bmatrix} \quad (23\text{-}48)$$

$$G_v = \begin{bmatrix} 0 \\ \tau^+_{zx} + \mu\tilde{S}_{zx} \\ \tau^+_{zy} + \mu\tilde{S}_{zy} \\ \tau^+_{zz} + \mu\tilde{S}_{zz} \\ Q_z + k\dfrac{\partial T^+}{\partial z} + \mu\,(\tilde{u}\tilde{S}_{zx} + \tilde{v}\,\tilde{S}_{zy} + \tilde{w}\,\tilde{S}_{zz}) \end{bmatrix} \quad (23\text{-}49)$$

Now the flux vector formulation, similar to that of the Navier-Stokes equation given by (14-1), is written as

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z} \quad (23\text{-}50)$$

The subgridscale terms τ^+_{ij} and Q_i are typically expressed in terms of the eddy viscosity and eddy diffusivity similar to that in RANS equations and is presented next.

23.2.2 Subgridscale Models

At this point, certain parallelisms between LES and RANS can be realized. Since a relatively strong background on RANS and turbulence models has already