Chapter 1

Turbulence Simulation

1.1 Navier-Stokes equations

Turbulent flows are always characterized by an unsteady and three-dimensional behaviour and can be described by the Navier-Stokes equations.

For a compressible flow, if a thermally and calorically perfect gas is considered and if the body forces are absent or negligible, the governing equations may be written as (Einstein notation used):

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} &= 0, \\
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} &= -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}, \\
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho E u_j)}{\partial x_j} &= -\frac{\partial (pu_j)}{\partial x_j} + \frac{\partial (u_j \sigma_{ij})}{\partial x_i} - \frac{\partial q_j}{\partial x_j}, \\
p &= \rho RT, \\
E &= C_v T + \frac{1}{2} u_i u_i. \quad (1.1)
\end{align*}
\]

In the above equations density, temperature, pressure, total energy for unit mass and specific heat at constant volume are represented respectively by \( \rho \), \( T \), \( p \), \( E \) and \( C_v \). In the last equation \( R \) is equal to \( \mathcal{R}/m \) where \( \mathcal{R} \) is the universal constant of perfect gas and \( m \) is the mole mass. By assuming the
flow to be Newtonian and under the Stokes hypothesis, the viscous stress tensor results:

$$\sigma_{ij} = \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$ (1.2)

where $\delta_{ij}$ is the kronecker delta and the viscosity coefficient $\mu$ is, generally, a function of the temperature. Moreover, the Fourier law is adopted to model the heat flux:

$$q_i = -K \frac{\partial T}{\partial x_i}$$ (1.3)

where $K$ is the conduction coefficient for the gas and is generally a function of the temperature. The system of equations quoted above can be numerically integrated for every turbulent flow providing a sufficiently fine spatial and temporal resolution. Because of the non-linearities of the equation system, the problem is characterized by a large range of spatial and temporal turbulent scales which a function of Reynolds number. The kinetic turbulent energy is extracted by the largest scales of turbulence and then it is transferred to smaller and smaller scales to be eventually is dissipate d, as predicted by the Energy Cascade concept. A typical distribution of energy in a turbulent flow a function of the wave-number, $n$, which is inversely proportional to the spatial scale, is represented in Fig. 1.1.

Fig. 1.1 gives information about the mean-energy of the turbulent structures which have the same dimensions. These structures can be splitted in the following ranges:

- **energy-containing range**, which contains the largest vortical turbulent structures
- **inertial range** or **subrange**, which contains vortexes of intermediate dimensions
- **dissipation range**, which contains the smallest structures.
To estimate the characteristic time and the spatial dimensions of turbulence, the results of the *Universal Equilibrium Theory* of Kolmogorov [7] can be used. For homogeneous and isotropic turbulence, the spatial orders of magnitude of the largest scales, L, and of the smallest scale in the flow, $l_k$, are related as follows:

$$\frac{L}{l_k} = Re^{3/4} \quad (1.4)$$

where $Re = \frac{UL}{\nu}$ is the Reynolds number of the flow, based on L and on an integral velocity, which can be assumed similar to the velocity of the largest scales. The previous relation clearly shows that the separation between large and small scales increases with the Reynolds number. The largest scales of turbulence carry most of the turbulence kinetic energy so they are responsible of the turbulent transport. The smallest scales are responsible of most of the dissipation of kinetic energy, so even if their contribution to the kinetic energy is negligible in comparison with the largest scales they must be considered to obtain accurate results. To this purpose, the single computational cell must have the dimensions of the smallest turbulent scales and the computational domain must be large enough to contain the largest flow structures. Thus, the number of nodes in the whole domain (N) increases with the Reynolds number.
number as follows:

\[ N = Re^{9/4}. \]  

(1.5)

As the Reynolds number increases, strong limitations for numerical simulation occur also due to the time resolution requirements. The governing equations, indeed, must be advanced for a global time interval, \( \Delta T_c \), of the order of the largest temporal scales, \( T_c \), and the temporal step must be small enough to capture the smallest temporal scales, of the order of \( t_k \). The ratio between the largest and the smallest temporal scales necessary to simulate the flux is clearly \( Re \) dependent:

\[ \frac{T_c}{t_k} = Re^{1/2}. \]  

(1.6)

Thus, if the global time step is constant, the number of temporal steps needed to cover all the range \( \Delta T_c \) quickly increases, as the Reynolds number is increased.

The huge computational resources needed to directly simulate turbulent flows at high Reynolds numbers (\( Re > 10^4 \)) are not affordable at present. For this reason, the direct numerical simulation (DNS) is only used for low Reynolds number flows in simple geometries. On the other hand the information which can be obtained in DNS, is much larger than the one required in industrial or engineering problems. Thus, other simplified models have been developed in order to obtain the required information at a significantly reduced computational cost. Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) are examples of these models.

It is important to stress, however, that DNS permits to obtain a large amount of information on turbulence, which is useful to devise and validate turbulent models for the closure of RANS and LES. Thus, DNS plays an important role for the industrial numerical simulation, although indirect.
1.2 Large Eddy Simulation

The large-eddy simulation approach (LES) is intermediate between DNS, where all fluctuations are resolved, and the statistical simulations based on RANS, where only the mean flow is simulated. In LES the severe Reynolds number restrictions of DNS are bypassed by directly simulating the large scales (GS) only and supplying the effect of the missing small scales (SGS) by a so-called sub-grid model. This is obtained by filtering the Navier-Stokes equations in space, in order to eliminate the flow fluctuations smaller than the filter size. In this way, the new unknowns of the problem become the filtered flow variables. Like for RANS, due to the non-linearity of the original problem, the new equations contain additional unknown terms, the so-called sub-grid scale (SGS) terms, representing the effect of the eliminated small scales on the filtered equations. In order to close the problem, these terms must be modelled. However, due to the fact that the small unresolved scales are often simpler in nature than the inhomogeneous large motions and do not significantly depend on the large scale motion, rather simple closure models may work well for many applications. Another advantage of this method is the possibility of directly simulating the largest scales, which are usually more interesting from the engineering point of view. Computationally, LES clearly is less demanding than DNS, but in general much more expensive than RANS. The reason is that, independently of the problem to be simulated, LES always requires fully three-dimensional and unsteady calculations even for flows which are two-dimensional and steady in the mean. Moreover LES, like DNS, needs to be carried out for long periods of time to obtain significant statistics. For these reasons, LES should provide better results for the analysis of complex three-dimensional and time-dependent problems for which the RANS approach frequently fails, in particular when large flow separation is present.

The use of LES for engineering problems is still not very extensive, but in the last years the interest in this method has largely increased.
1.2.1 SGS modeling

The energy-containing large scale structures (GS) mainly contribute for the turbulent transport while the dissipative small scale motions (SGS) carry most of the vorticity and act as a sink of turbulent kinetic energy. For high Reynolds numbers the dissipative part of the spectrum becomes clearly separated from the low wave-number range, in a way shown by Eq. (1.4). Some of the significant differences between GS and SGS scales are summarised in Tab. 1.1, Ref. [5].

To illustrate the role of SGS models, it is useful to consider possible con-

<table>
<thead>
<tr>
<th>GS turbulence</th>
<th>SGS turbulence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Produced by mean flow</td>
<td>Produced by larger eddies</td>
</tr>
<tr>
<td>Depends on boundaries</td>
<td>Universal</td>
</tr>
<tr>
<td>Ordered</td>
<td>Chaotic</td>
</tr>
<tr>
<td>Requires deterministic description</td>
<td>Can be modelled statistically</td>
</tr>
<tr>
<td>Inhomogeneous</td>
<td>Homogeneous</td>
</tr>
<tr>
<td>Anisotropic</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Long-lived</td>
<td>Short-lived</td>
</tr>
<tr>
<td>Diffusive</td>
<td>Dissipative</td>
</tr>
<tr>
<td>Difficult to model</td>
<td>Easier to model</td>
</tr>
</tbody>
</table>

Table 1.1. Qualitative differences between GS turbulence and SGS turbulence

sequences if turbulent simulation are performed with insufficient resolution. In this case the viscous dissipation in the flow cannot properly be accounted for. This will typically result in an accumulation of energy at the high wave-number end of the spectrum which reflects a distorted equilibrium state between production and dissipation of turbulent kinetic energy. For sufficiently high Reynolds numbers (or sufficiently coarse grids) the discrete representation of the flow becomes essentially inviscid and the non-linear transfer of energy can lead to an unbounded growth of turbulence intensities and eventually to numerical instability of the computation.
1.2.2 Filtered equations of the motion

In LES any dependent variable of the flow, \( f \), is split into a GS part, \( \overline{f} \), and a SGS part, \( f' \):

\[
f = \overline{f} + f'
\]  

(1.7)

Generally, the GS component, \( \overline{f} \), represents that part of the turbulent fluctuation which remains after some smoothing which has been applied to the flow field.

For compressible flows, it is convenient to define a density weighted filter since it allows to partially recover the formal structure of the equations of the incompressible problem. This filter is defined as in Eq. (1.8)

\[
\tilde{f} = \frac{\rho f}{\rho}.
\]  

(1.8)

Applying the filtering operation to the Navier-Stokes equations, Eq. (1.1), yields the equations of motion of the GS flow field. Like in RANS the filtering of the non linearities is of particular interest since it gives rise to additional unknowns terms. For LES of compressible flows, the filtered form of the equations of motion for a thermally and calorically perfect gas is the following:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \bar{u}_j)}{\partial x_j} = 0
\]

\[
\frac{\partial (\rho \bar{u}_i)}{\partial t} + \frac{\partial (\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial \rho}{\partial x_i} + \frac{\partial (\mu \bar{P}_{ij})}{\partial x_j} - \frac{\partial M_{ij}^{(1)}}{\partial x_j} + \frac{\partial M_{ij}^{(2)}}{\partial x_j}
\]

\[
\frac{\partial (\rho \bar{E})}{\partial t} + \frac{\partial (\rho \bar{E} + \rho \bar{u}_i \bar{u}_j)}{\partial x_j} = \frac{\partial (\bar{u}_i \bar{u}_{ij})}{\partial x_i} - \frac{\partial \bar{q}_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left( Q_{ij}^{(1)} + Q_{ij}^{(2)} + Q_{ij}^{(3)} \right)
\]  

(1.9)

In the momentum equation the sub-grid terms are represented by the terms \( M_{ij}^{(i)} \) which can be defined as follows:
\[ M_{ij}^{(1)} = \rho u_i u_j - \rho \hat{u}_i \hat{u}_j \] (1.10)
\[ M_{ij}^{(2)} = \mu P_{ij} - \mu \hat{P}_{ij} \] (1.11)

where \( P_{ij} \) is defined in Eq.1.12.
\[ P_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \] (1.12)
\[ p = \rho RT, \] (1.13)
\[ \bar{e} = C_v \bar{T}, \] (1.14)

\( M_{ij}^{(1)} \) takes into account the momentum transport of the sub-grid scales and \( M_{ij}^{(2)} \) represents the transport of viscosity due to the sub-grid scales fluctuations.

In the energy equation the sub-grid term are represented by the terms \( Q_j \) which can be defined as follows:

\[ Q_j^{(1)} = \left[ \hat{u}_i \left( \rho \hat{E} + p \right) - u_i (\rho E + p) \right] \] (1.15)
\[ Q_j^{(2)} = \left( \mu P_{ij} \hat{u}_j \right) - \left( \mu \hat{P}_{ij} \hat{u}_j \right) \] (1.16)
\[ Q_j^{(3)} = K \frac{\partial T}{\partial x_j} - K \frac{\partial \bar{T}}{\partial x_j} \] (1.17)

\( Q_j^{(1)} \) represents three distinct physical effects:
- the transport of energy \( E \) due to small scales fluctuations;
- the change of the internal energy due to the sub-grid scale compressibility \( \left( p \frac{\partial u_i}{\partial x_j} \right) \);
- the dissipation of energy due to sub-grid-scale motions in the pressure field \( \left( u_j \frac{\partial p}{\partial x_j} \right) \);

\( Q_j^{(2)} \) takes in account the dissipative effect due to the sub-grid scale transport of viscosity; \( Q_j^{(3)} \) takes in account the heat transfer caused by the motion of the neglected sub-grid scales.
1.2.3 Subgrid Scale model

Smagorinsky model

The Smagorinsky model is an example of closure models (ref.[8]). We assume that low compressibility effects are present in the SGS fluctuations and that heat transfer and temperature gradients are moderate. The retained SGS term in the momentum equation is thus the classical SGS stress tensor:

\[ M_{ij} = \rho \bar{u}_i \bar{u}_j - \bar{\rho} \bar{u}_i \bar{u}_j \]  

(1.18)

where the over-line denotes the grid filter and the tilde the density-weighted Favre filter (Eq.1.8). The isotropic part of \( M_{ij} \) can be neglected under the assumption of low compressibility effect in the SGS fluctuations. The deviatoric part, \( T_{ij} \), may be expressed by an eddy viscosity term, in accordance with the Smagorinsky model extended to compressible flow:

\[ T_{ij} = -2 \mu_s \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \right), \]  

(1.19)

\[ \mu_s = \bar{\rho} C_s \Delta^2 |\tilde{S}|, \]  

(1.20)

where \( \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \) is the resolved strain rate tensor, \( \mu_s \) is the SGS viscosity, \( \Delta \) is the filter width, \( C_s \) is a constant which must be assigned a priori and \( |\tilde{S}| = \sqrt{\tilde{S}_{ij} \tilde{S}_{ij}} \). The width of the filter is defined for every grid elements, \( i \), as follows:

\[ \Delta^{(i)} = V ol_j^{1/3} \]  

(1.21)

where \( V ol_j \) is the volume of the \( j^{th} \) grid element.

In the energy equation the effect of the SGS fluctuations has been modified by the introduction of a constant SGS Prandtl number to be assigned a priori:

\[ Pr_{sgs} = C_p \frac{\mu_s}{K_{sgs}} \]  

(1.22)
where $K_{sgs}$ is the SGS conductivity coefficient and it takes into account the diffusion of total energy caused by the SGS fluctuation. In the filtered energy equation, the term $K_{sgs}$ is added to the molecular conductivity coefficient. Experiments pointed out that a $C_s$ constant value brings a lot of problems, like a wrong asymptotic behaviour in the near wall region ($\tau_{ij}$ different from zero) and the impossibility of turbulent energy transfer from small to large scales, because the first ones have only the effect of dissipating energy. This problem has been partially overcome with the introduction of a dynamic version of Smagorinsky model, in which $C_s$ is locally obtained using the smallest scales computed. This dynamic procedure is based on a particular algebraic identity and on the use of a test filter coarser than the one used to filter Navier Stokes equations (Germano et al., 1991). This approach eliminates most of the problems of a static eddy viscosity model closure, although numerical instability may appear due to high fluctuations of the $C_s$ coefficient that may bring to a local negative viscosity.

Another way to obtain the correct asymptotic behaviour in the near wall region is to use different expression of the SGS viscosity. The Vreman and WALE model are examples of such subgrid-scale closures.

**Vreman model**

The Vreman model [2] is designed with first-order derivatives and thus is not more complicated than the Smagorinsky model. This model is designed to give a zero eddy viscosity when zero theoretical value is expected and to adapt to the local level of turbulent activity, while it does not need more than the local filter width and the first-order derivatives of the velocity field.

The eddy viscosity $\mu_v$ of the Vreman model is defined by:

$$\mu_v = c\left(\frac{B_\beta}{\alpha_{ij}^\alpha_{ij}}\right)^{\frac{1}{2}}$$

with

$$\alpha_{ij} = \partial \tilde{u}_j / \partial x_i$$
\( \beta_{ij} = \Delta^2 \alpha_{mi} \alpha_{mj} \)

\[ B_\beta = \beta_{11}\beta_{22} - \beta_{12}^2 + \beta_{11}\beta_{33} - \beta_{13}^2 + \beta_{22}\beta_{33} - \beta_{23}^2 \]

The constant \( c \approx 2.5 C_s^2 \) where \( C_s \) denotes the Smagorinsky constant.

The Vreman SGS model has been validated first on a transitional and turbulent mixing layer at high Reynolds number and then on a turbulent channel flow at \( Re_\tau = 360 \). An appropriate transitional and near-wall flow behaviour was found with this model which, moreover seems to be robust in high Reynolds number simulations.

It has been also shown to be more accurate than the Smagorinsky model in homogeneous turbulence.

**WALE model**

The Wall-Adapting Local Eddy-Viscosity (WALE) SGS model proposed by Nicoud and Ducros [3] is based on the square of the velocity gradient tensor. Improvements compared to the classical Smagorinsky model are firstly the property to give a zero value of the eddy-viscosity near a wall without using a dynamic procedure, then to produce zero eddy-viscosity in case of a pure shear and finally the property to detect all the turbulence structures relevant for the kinetic energy dissipation.

The eddy-viscosity term \( \mu_w \) of the model is defined by:

\[
\mu_w = C_w \Delta^2 \frac{\left( \overline{S_{ij}^d \overline{S_{ij}^d}} \right)^{\frac{3}{4}}}{(S_{ij} S_{ij})^{\frac{3}{4}} + (S_{ij}^d S_{ij}^d)^{\frac{3}{4}}} \tag{1.24}
\]

with

\[
\overline{S_{ij}^d} = \frac{1}{2} (\overline{g_{ij}^2} + \overline{g_{ji}^2}) - \frac{1}{3} \frac{\delta_{ij}}{\overline{g_{kk}^2}}
\]

is the symmetric part of the tensor \( \overline{g_{ij}^2} = \overline{g_{ik}g_{kj}} \), where \( \overline{g_{ij}} = \partial \tilde{u}_i / \partial x_j \)

and in which the constant \( C_w \) is set to 0.1.

The performance of the WALE model has been in particular illustrated for a freely decaying isotropic turbulence and for a turbulent pipe flow using a hybrid mesh [3].