Chapter 8

Introduction to Modelling and Simulation

8.1 The Challenge

In the study of turbulent flows—as in other fields of scientific inquiry—the ultimate objective is to obtain a tractable quantitative theory or model that can be used to calculate quantities of interest and practical relevance. A century of experience has shown the "turbulence problem" to be notoriously difficult, and there are no prospects of a simple analytic theory. Instead, the hope is to use the ever-increasing power of digital computers to achieve the objective of calculating the relevant properties of turbulent flows. In the subsequent chapters, five of the leading computational approaches to turbulent flows are described and examined.

It is worthwhile at the outset to reflect on the particular properties of turbulent flows that make it difficult to develop an accurate tractable theory or model. The velocity field $\mathbf{U}(\mathbf{x}, t)$ is three-dimensional, time-dependent and random. The largest turbulent motions are almost as large as the characteristic width of the flow, and consequently are directly affected by the boundary geometry (and hence are not universal). There is a large range of timescales and lengthscales. Relative to the largest scales, the Kolmogorov timescale decreases as $\mathrm{Re}^{-\frac{1}{2}}$, and the Kolmogorov lengthscale as $\mathrm{Re}^{-\frac{3}{4}}$. In wall-bounded flows, the most energetic motions (that are responsible for the peak turbulence production) scale with the viscous lengthscale δ_ν which is small compared to outer scale δ, and which decreases (relative to δ) approximately as $\mathrm{Re}^{-0.8}$.

Difficulties arise from the non-linear convective term in the Navier-Stokes

equations, and much more so from the pressure-gradient term. When expressed in terms of velocity (via the solution to the Poisson equation, Eq. 2.49 on page 21) the pressure-gradient term is both non-linear and non-local.

8.2 Overview of Approaches

The methodologies described in the subsequent chapters take the form of sets of partial differential equations, in some cases supplemented by algebraic equations. For a given flow, with the specification of the appropriate initial and boundary conditions, these equations are solved numerically.

In a turbulent flow *simulation*, equations are solved for a time-dependent velocity field which, to some extent, represents the velocity field $\mathbf{U}(\mathbf{x}, t)$ for one realization of the turbulent flow. In contrast, in a *turbulence model*, equations are solved for some mean quantities, for example $\langle \mathbf{U} \rangle$, $\langle u_i u_j \rangle$ and ε. (The word "models" is used to refer to both simulations and turbulence models, when the distinction is not needed.)

The two simulation approaches described are direct numerical simulation (DNS, Chapter 9), and large-eddy simulation (LES, Chapter 13). In DNS, the Navier-Stokes equations are solved to determine $\mathbf{U}(\mathbf{x}, t)$ for one realization of the flow. Because all lengthscales and timescales have to be resolved, DNS is computationally expensive; and, because the computational cost increases as Re^3, this approach is restricted to low-to-moderate Reynolds number flows. In LES, equations are solved for a "filtered" velocity field $\overline{\mathbf{U}}(\mathbf{x}, t)$, which is representative of the larger-scale turbulent motions. The equations solved include a model for the influence of the smaller-scale motions which are not directly represented.

The approaches described in Chapters 10 and 11 are called RANS (Reynolds-averaged Navier-Stokes), since they involve the solution of the Reynolds equations to determine the mean velocity field $\langle \mathbf{U} \rangle$. In the first of these approaches, the Reynolds stresses are obtained from a turbulent viscosity model. The turbulent viscosity can be obtained from an algebraic relation (as in the mixing-length model) or it can be obtained from turbulence quantities such as k and ε for which modelled transport equations are solved. In Reynolds-stress models (Chapter 11), modelled transport equations are solved for the Reynolds stresses, thus obviating the need for a turbulent viscosity.

The mean velocity $\langle \mathbf{U} \rangle$ and the Reynolds stresses $\langle u_i u_j \rangle$ are the first and second moments of the Eulerian PDF of velocity $f(\mathbf{V}; \mathbf{x}, t)$. In PDF methods (Chapter 12), a modelled transport equation is solved for a PDF

such as $f(\mathbf{V}; \mathbf{x}, t)$.

8.3 Criteria for Appraising Models

The purpose of this section is to provide an overview of the criteria used in appraising models.

Historically, many models have been proposed and many are currently in use. It is important to appreciate that there is a broad range of turbulent flows, and also a broad range of questions to be addressed. Consequently it is useful and appropriate to have a broad range of models, that vary in complexity, accuracy, and other attributes.

The principal criteria that can be used to assess different models are

(i) Level of description

(ii) Completeness

(iii) Cost and ease of use

(iv) Range of applicability

(v) Accuracy

As examples to elaborate on these criteria, we consider two models—the mixing-length model and DNS—which are at the extremes of the range of approaches.

Recall that DNS (direct numerical simulation) consists of solving the Navier-Stokes equations to determine the instantaneous velocity field $\mathbf{U}(\mathbf{x}, t)$ for one realization of the flow. The mixing-length model (applied to statistically-stationary two-dimensional boundary-layer flows) consists of the boundary-layer equations for $\langle U(x,y)\rangle$ and $\langle V(x,y)\rangle$, with the Reynolds shear stress and the turbulent viscosity being obtained from the model equations

$$\langle uv\rangle = -\nu_T \frac{\partial\langle U\rangle}{\partial y}, \tag{8.1}$$

and

$$\nu_T = \ell_m^2 \left|\frac{\partial\langle U\rangle}{\partial y}\right|. \tag{8.2}$$

The mixing length $\ell_m(x,y)$ is specified as a function of position.

Level of Description. In DNS, the flow is described by the instantaneous velocity $\mathbf{U}(\mathbf{x}, t)$, from which all other information can be determined. For example, flow visualizations can be performed to examine turbulent structures,

and multi-time, multi-point statistics can be extracted. In the mixing-length model, on the other hand, the description is at the mean-flow level: apart from the specified mixing length, the only quantities represented directly are $\langle U \rangle$ and $\langle V \rangle$. No information is provided about PDF's of velocity, two-point correlations, or turbulence structures, for example. The limited description provided by mean-flow closures (such as the mixing-length model) *is adequate* in many applications. The issue is more that a higher level of description can provide a more complete characterization of the turbulence, leading to models of greater accuracy and wider applicability.

Completeness. A model is deemed complete if its constituent equations are free of flow-dependent specifications. One flow is distinguished from another solely by the specification of material properties (i.e., ρ and ν) and of initial and boundary conditions. DNS is complete, whereas the mixing-length model is incomplete: the mixing length $\ell_m(x, y)$ has to be specified, and the appropriate specification is flow dependent.

Incomplete models can be useful for flows within a narrow class (e.g., attached boundary layers on airfoils) for which there is a body of semi-empirical knowledge on the appropriate flow-dependent specifications. But in general, completeness is clearly desirable.

Cost and Ease of Use. In all but the simplest of flows, numerical methods are required to solve the model equations. The difficulty of performing a turbulence-model calculation depends both on the flow and on the model.

Table 8.1 provides a categorization of turbulent flows according to their geometry. The computational difficulty increases with the statistical dimensionality of the flow: it decreases if the flow is statistically stationary, and decreases further if boundary-layer equations can be used.

In some approaches (e.g., DNS) the computational cost is a rapidly increasing function of the Reynolds number of the flow; whereas in others (e.g., mixing length) the increase in cost with Reynolds number is insignificant or non-existent.

The task of performing a turbulent flow calculation for a particular flow can be considered in two parts. First, the computer program to solve the model equations has to be obtained or developed, and set up for the flow at hand (e.g., by specifying appropriate boundary conditions). Second, the computer program is executed to perform the calculation, and the required results are extracted. The cost and difficulty of the first step depends on the available software and algorithms, and on the complexity of the model. The effort required to develop a computer program for a particular class of flows and models can be very significant, and is therefore a substantial impediment

Table 8.1: Examples of turbulent flows of different computational difficulty. The difficulty increases downwards and to the right.

Dimensionality number of directions of statistical inhomogeneity	**Boundary Layer** statistically stationary, boundary-layer approximations apply	**Statistically Stationary**	**Not Statistically Stationary**
OD			homogeneous shear flow
1D		fully-developed pipe or channel flow; self-similar free shear flows[a]	temporal mixing layer
2D	flat-plate boundary layer; jet in a co-flow	flow through a sudden expansion in a 2D duct	flow over an oscillating cylinder
3D	boundary layer on a wing	jet in a cross-flow; flow over an aircraft or building	flow in the cylinder of a reciprocating engine

[a]In similarity variables, turbulence-model equations for 2D self-similar free shear flows have a single independent variable.

to the evaluation and use of new models requiring new programs. It is, however, a "one-time cost".

The cost and difficulty of the second part—performing the computation—depends on the scale of computer required (e.g., workstation or supercomputer), on the amount of human time and skill needed to perform the computation, and on the computer resources consumed. These are "recurrent costs."

In terms of computer time consumed, what computational cost is acceptable? The answer can vary by a factor of a million, depending on the context. Peterson et al. (1989) suggest that about 200 hours of CPU time on the most powerful supercomputers is the upper reasonable limit on "large-scale research" calculations. (The channel-flow DNS of Kim et al. 1987 required 250 hours.) Very few calculations of this scale are performed. For "applications" Peterson et al. (1989) suggest that a more reasonable time is 15 minutes CPU time on the most powerful supercomputers, which corresponds to 25 hours of CPU time on a workstation of one hundredth the speed. To perform engineering design studies on a workstation—requiring "repetitive"

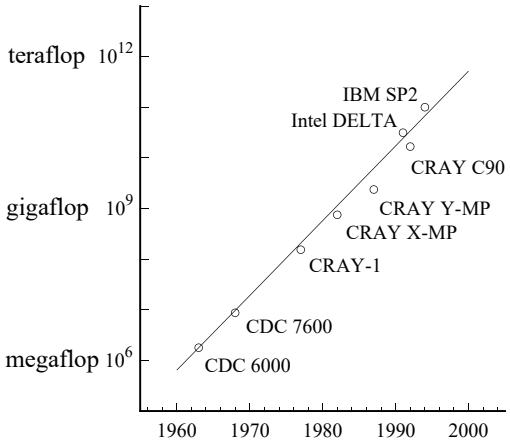

Figure 8.1: Speed (*flops* per second) of the fastest supercomputers against the year of their introduction. The line shows a growth rate of a factor of 30 per decade. (Adapted from Foster 1995.)

turbulent flow calculations—CPU times of a minute or less per calculation are desirable. The ratio between the sizes of these "repetitive," "application" and "large-scale research" computations is $1 : 1.5 \times 10^3 : 1.2 \times 10^6$.

The amount of computation measured in *flops* (floating-point operations) that can be performed in a given time is determined by the speed of the computer, measured in *megaflops*, *gigaflops* or *teraflops*, i.e., $10^6, 10^9$ or 10^{12} flops per second.[1] Figure 8.1 shows the peak speed of the largest supercomputers over a 30 year period. It may be seen that the speed has increased exponentially, by a factor of 30 per decade. This is a remarkable rate of increase—a factor of a thousand in 20 years, and a million in 40 years. While there is no sound basis for extrapolation beyond a few years, it is nevertheless generally supposed that this trend will continue (Foster 1995). Consequently, today's "research" approaches may be feasible for "applications" in 20 years, and for "repetitive" calculations in 40 years. On the other hand, this forty-year span between "large-scale research" and "repetitive" computations again illustrates the need for a range of models, differing in their computational requirements.

(The absolute speeds shown on Fig. 8.1 need to be viewed with caution. The speed achieved in practice may be less than the peak speed by one or even two orders of magnitude. Typically only a fraction (e.g., one eighth) of the processors of a parallel computer are used, and only 20–50% of the

[1]Note that *flops* is number of operations, whereas *megaflops* is a rate, i.e., number of operations (in millions) per second.

peak speed is achieved on each processor. It should also be appreciated that, while here the focus of the discussion is on CPU time, memory can also be a limiting factor.)

Range of Applicability. Range of Applicability Not all models are applicable to all flows. For example, there are many models based on velocity spectra or two-point correlations, which are applicable only to homogeneous turbulence. (Such models are not considered here, but are described in the books of Lesieur 1990 and McComb 1990.) As a second example, particular mixing-length models typically make assumptions about the flow geometry in the specification of the mixing length, so that their applicability is confined to flows of that geometry. Computational requirements place another—though nonetheless real—limitation on the applicability of some models. In particular, for DNS the computational requirements rise so steeply with Reynolds number that the approach is applicable only to flows of low or moderate Reynolds number. This limitation is examined in more detail in Chapter 9.

In this book, attention is focused on the velocity field in constant-density flows. It should be appreciated, however, that in many flows to which turbulence models are applied there are additional phenomena, such as heat and mass transfer, chemical reactions, buoyancy, compressibility, and multiphase flow. An important consideration, therefore, is the extent to which the approaches considered here are applicable to—or can be extended to—these more complex flows.

It is emphasized that in these considerations we separate *applicability* from *accuracy*. A model is applicable to a flow if the model equations are well-posed and can be solved, whether or not the solutions are accurate.

Accuracy. It goes without saying that accuracy is a desirable attribute of any model. In application to a particular flow, the accuracy of a model can be determined by comparing model calculations with experimental measurements. This process of model testing is of fundamental importance and deserves careful consideration. As shown in Fig. 8.2, the process consists of a number of steps, several of which introduce errors.

For a number of reasons, the boundary conditions in the calculations may not correspond exactly to those of the measured flow. A flow may be approximately two-dimensional, but may be assumed to be exactly so in the calculations. Boundary conditions on some properties may not be known, and so have to be estimated; or, they may be taken from experimental data which contain some measurement error.

The numerical solution of the model equations inevitably contains nu-

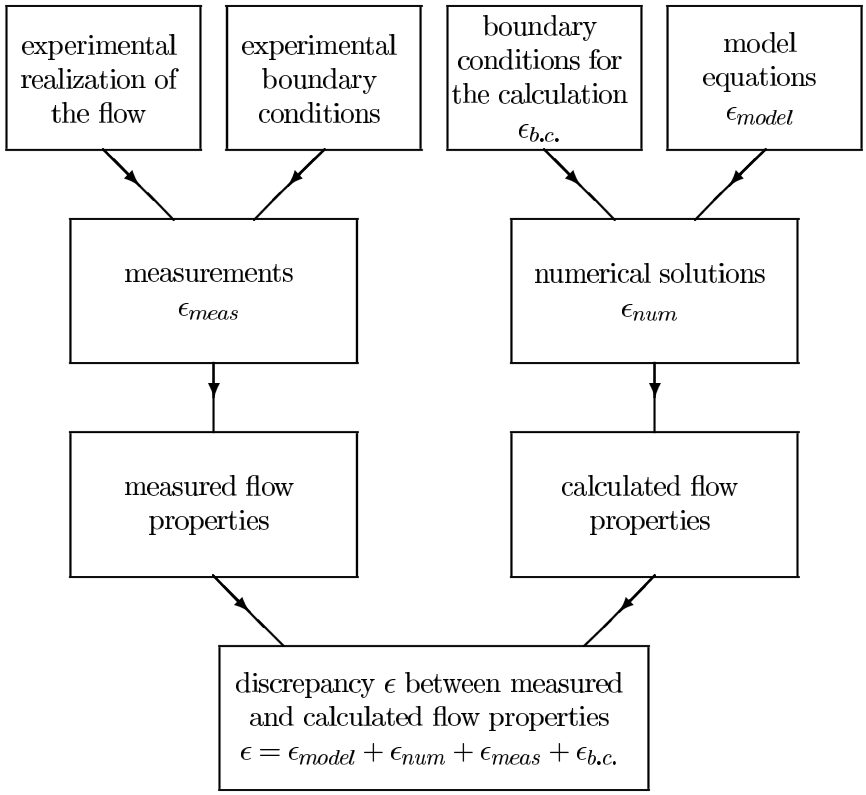

Figure 8.2: Chart illustrating that the discrepancy ϵ between measured and calculated flow properties stem from: model inaccuracies, ϵ_{model} ; numerical errors, ϵ_{num}; measurement errors ϵ_{meas}; and from discrepancies in the boundary conditions, $\epsilon_{\text{b.c.}}$. (The equation given for ϵ is merely suggestive: the errors do not add linearly.)

merical error. This may be from a number of sources, but it is often dominated by spatial truncation error. In a finite-difference or finite-element method, for example, this error scales as a positive power of the grid spacing, Δx, while the computational cost increases with $1/\Delta x$—possibly as a positive power. Many published turbulence-model calculations contain significant numerical errors, either because the available computer resources do not allow a sufficiently fine grid spacing, or, put bluntly, because the calculations are performed with insufficient care or regard for numerical accuracy.

In summary, as depicted in Fig. 8.2, the discrepancy between measured and calculated flow properties arise from

(i) inaccuracies of the model

(ii) numerical error

(iii) measurement error

(iv) discrepancies in the boundary conditions.

The important conclusion is that a comparison between measured and calculated flow properties determines the accuracy of the model only if the errors arising from (ii)–(iv) are relatively small. In particular, there is a danger of drawing false conclusions about model accuracy from calculations containing large or unquantified numerical errors. These issues are discussed further by Coleman and Stern (1997).

Final Remarks. The suitability of a particular model for a particular turbulent flow problem depends on a weighted combination of the criteria discussed above; and the relative weighting of importance of the different criteria depends significantly on the problem. Consequently, as mentioned at the outset, now and into the future, there is not one "best" model, but rather there is a range of models that can usefully be applied to the broad range of turbulent flow problems.