Introduction

Fernando F. Grinstein, Len G. Margolin, and William J. Rider

The numerical simulation of turbulent fluid flows is a subject of great practical importance to scientists and engineers. The difficulty in achieving predictive simulations is perhaps best illustrated by the wide range of approaches that have been developed and that are still being used by the turbulence modeling community. In this book, we describe one of these approaches, which we have termed *implicit large eddy simulation* (ILES).

ILES is remarkable for its simplicity and general applicability. Nevertheless, it has not yet received widespread acceptance in the turbulence modeling community. We speculate that this is the result of two factors: the lack of a theoretical basis to justify the approach and the lack of appreciation of its large and diverse portfolio of successful simulations. The principal purpose of this book is to address these two issues.

One of the complicating features of turbulence is the broad range of spatial scales that contribute to the flow dynamics. In most examples of practical interest, the range of scales is much too large to be represented on even the highest-performance computers of today. The general strategy, which has been employed successfully since the beginning of the age of computers, is to calculate the large scales of motion and to introduce models for the effects of the (unresolved) small scales on the flow. In the turbulence modeling community, these are called *subgrid-scale (SGS) models*.

In ILES, we dispense with explicit subgrid models. Instead, the effects of unresolved scales are incorporated implicitly through a class of nonoscillatory finite-volume (NFV) numerical fluid solvers. This class includes such well-known methods as flux-corrected transport (FCT), the piecewise parabolic method (PPM), and total variation diminishing (TVD) algorithms. In general, NFV methods have been a mainline methodology in the computational fluid dynamics community for more than 30 years. However, the recognition of the ILES property is much more recent.

The opening section of the book, Motivation, recounts the early history of ILES and proposes a rationale for the approach. One can imagine the initial resistance of the turbulence modeling community, for whom the creation of new and more complex subgrid-scale models has become its *raison d'etre*. Further, this community has historically emphasized the importance of distinguishing physical model from numerical error, leading to the belief that NFV methods are inappropriate for turbulence modeling. One should also realize that the earliest pioneers of ILES worked in relative isolation, being unaware of each other's work. This made it difficult to identify the essential elements of the ILES approach and to develop a physical justification.

More recently, it has been recognized that the ILES property originates in the blurring of the boundaries between physical modeling and numerical approximation. This is the subject of the second section of the book, Capturing Physics with Numerics, where the idea of building physics into numerical methods is developed. To be precise, NFV methods implement the mathematical property of preserving monotonicity into the integral form of the governing equations. This leads to a computable model in which energy is dissipated on the resolved scales of the simulation at the physically correct rate, due to the inertially dominated processes involved. In this section, we describe several concepts that lead to NFV approximations. We also explore the relationship between ILES and more conventional subgrid-scale models.

The most compelling argument for ILES lies in the diversity of its portfolio of successful applications. In the third section, Verification and Validation, we collect many results aimed at verifying and validating our models by comparison with theory and experiment. The engineering and laboratory experiments range in Reynolds number (Re) from several hundreds to several tens of thousands. The simulations in this section depend on a variety of NFV methods; our purpose here is to demonstrate the underlying generality of ILES, rather than to distinguish among different NFV methods.

In the fourth and final section, Frontier Flows ($Re > 10^6$), we offer examples of more complex simulations for which there are, at present, little on no data available for validation. In principle, the lack of parameters of the ILES approach implies the increased generality and predictive capabilities of the ILES approach. In practice, we believe it is important to quantify the limits of applicability of this approach by continuing with testing and making efforts to understand its foundations.

Section A: Motivation

In Chapter 1, Jay Boris, the originator and first proponent of the ILES approach, recounts his early development of monotone integrated LES (MILES), which is the monotonicity-preserving version of the ILES approach. He reflects on the initial reactions of the traditional turbulence modeling community to his work. In Chapter 2, we introduce our survey of ILES methods with a synthesis of the main components of our current theoretical understanding of ILES for the simulation of turbulent flows. We emphasize the importance of numerical methods that are built upon a physical understanding and are not simply numerical approximations. In fact, the best numerical approximations encode a substantial amount of physics directly into the integration procedures. This recognition is a key to further progress in modeling complex turbulent flows through ILES.

Section B: Capturing physics with numerics

Whenever a physical system is modeled computationally, the desire is to represent the physical world with as much fidelity as possible. One of the key aspects of achieving this goal is the physical modeling that is numerically integrated. The methods described in this book are no different, but the approach to achieving this goal is.

Rather than separate the physical modeling from the numerical integration, the two enterprises are conducted simultaneously. We can refer to this as *capturing physics*, which we regard as a natural extension of the idea of shock capturing. We prefer this approach because it circumvents the problem of first composing a model and then worrying about integrating it successfully. The model and the integration are seamlessly coupled, and the basic issues of numerical stability and model consistency are handled as a matter of course.

In the following chapters these basic ideas are expanded upon in a sequence of expositions that describe the basic models and their physical basis, their basic mathematical properties, their fundamental performance, and the details of the algorithms. In Chapter 3, Sagaut provides a whirlwind overview of the world of large eddy simulation (LES) modeling of which ILES is but a part. The presentation begins with a discussion of the derivation of the equations to be solved. Various approaches to conducting modeling and calculations are discussed. The basic requirements for LES methods and models are detailed, along with a description of the basic modeling approaches.

The description of the various methods used for ILES is presented in Chapter 4. The numerical methods for ILES are nonlinear and provide nonlinear stability for numerical integration. The analysis uncovers the models implicitly included through the utilization of these techniques. With the use of standard techniques in numerical analysis, the various methods are studied and classified, and their behavior is predicted. This produces a common perspective to view the methods and their relation to standard LES modeling.

Chapter 4a, by Drikakis et al. discusses the details of flux-limiting methods as used for ILES. This represents an enormous class of hybrid methods, including FCT and many TVD algorithms. This chapter focuses on the commonality of the various methods and their basic performance on turbulent flows, which is then demonstrated in a canonical test case that has been traditionally used to study transition and turbulence decay. This performance is related to the functional forms implicitly included through the nonlinear numerical algorithms. Modified equation analysis is used to show that the truncation error terms introduced by such methods provide implicit SGS models similar in form to those of conventional mixed SGS models.

One important class of methods for ILES consists of high-resolution Godunov-type methods. Chapter 4b, by Woodward, discusses one important method in this class, PPM. The basics of the piecewise constant and linear Godunov methods are introduced, followed by PPM. This introduction covers the basic method and more modern extensions that are particularly useful for modeling turbulent flows.

In the Lagrangian remap method by Youngs (Chapter 4c), a simple finite-difference formulation is used for a Lagrangian phase in conjunction with an accurate interface reconstruction method that is based on using a van Leer monotonic advection method. This relatively simple technique has been very successfully used for a wide range of complex problems, providing an effective way of calculating many relatively complex turbulent flows.

Many ILES models are distinquished by the physical insight that is inherent in their composition. Chapter 4d, by Smolarkiewicz and Margolin, explores algorithms that use different physical insights than other methods discussed in Chapters 4a and 4b. Despite these differences, the methods described in this chapter perform at a high level. The chapter also provides a guide to the aspects of these methods that are common among the other approaches.

The underlying idea of the vorticity confinement method presented in Chapter 4e is similar to that used in shock capturing, where intrinsically discrete equations are satisfied in thin, modeled regions. This direct, grid-based modeling approach is an effective alternative to formulating a partial differential equation model for the small-scale, turbulent vortical regions and then discretizing it.

A common framework for numerical regularization, analysis, and understanding of ILES is discussed in Chapter 5 by Rider and Margolin. The analysis provided is founded on the modified equation analysis technique, which produces a differential equation that the numerical method solves more accurately than the original differential equation. The prototypical example is the advection–diffusion equation produced by upwind differencing for a purely advection equation. In the case of modern high-resolution methods, the numerical method provides an effective differential equation that has many explicit LES models embedded implicitly in the solution technique. This approach also provides a rational approach to understanding ILES through the common language of continuum mechanics.

Approximate deconvolution is used in traditional LES modeling. Researchers have found that it provides a framework to connect traditional LES models to implicit models. Chapter 6, by Adams, Hickel, and Domaradzki, describes this technique and its power in connecting these two seemingly disparate approaches. Much of the machinery associated with modern high-resolution methods can be recast as an approximate deconvolution. This approach provides an effective bridge between many recent explicit LES models and a broad family of implicit models associated with ILES. This is based on the recognition that one must add physically realizable information to close a differential equation whether one is solving the equation through explicit modeling or a high-resolution numerical method. The approach described in Chapter 6 is an innovative contribution to this general approach.

Section C: Verification and validation

In this section we present results aimed at the verification and validation of ILES by comparison with analytic models of idealized turbulence, with direct numerical simulation of simple flows, or with laboratory studies, as appropriate. Implementation issues and examples of ILES for the simulation of turbulent flows of practical interest are also addressed in this section. The performance of the approach is demonstrated and assessed in a variety of fundamental engineering applications.

In Chapter 7, Porter and Woodward begin the section by presenting a detailed and systematic evaluation of ILES applications for canonical and simple flows for which direct numerical simulation data, theoretical data, or high-quality laboratory data are available. These flows include forced and decaying homogeneous isotropic turbulence.

Next, Chapters 8 and 9, by Grinstein and Drikakis, respectively, discuss new insights generated in ILES studies of the dynamics of high-Renolds-number flows driven by Kelvin–Helmholtz instabilities. The studies in Chapter 8 are relevant to global instabilities, vortex dynamics and topology governing the shear layer development, and transition to turbulence from laminar conditions. Chapter 9 examines symmetry breaking and nonlinear bifurcation phenomena, and shows that NFV numerical schemes exhibit a variety of behavior in the simulation of these phenomena, depending on the nonlinear dissipation and dispersion properties of the particular scheme.

The application of ILES in the study of wall-bounded flows is addressed in Chapters 10 and 11. In Chapter 10 Fureby et al. first discuss the application of ILES to incompressible flows such as (i) fully developed turbulent channel flows, (ii) flow over a cylinder, (iii) flow over a sudden expansion, (iv) flow over a surface-mounted cube, and (v) the flow past a prolate spheroid at different angles of attack. Next, in Chapter 11, Fureby and Knight discuss the ILES applications in compressible bounded turbulent shear flow regimes. Issues associated with the computational grid are discussed, including requirements for resolution of the turbulence production mechanism in the viscous sublayer. The implications of scaling LES to higher Reynolds numbers are addressed. Specific applications are presented, including compressible adiabatic and isothermal zero-pressure-gradient boundary layers and shock wave boundary layers. The extension of these techniques to general compressible bounded shear flows is discussed, and examples such as the supersonic base flow are presented.

ILES based on vorticity confinement is examined by Steinhoff et al. in Chapter 12. The method is especially well suited to treat flow over blunt bodies, including attached and separating boundary layers, and resulting turbulent wakes. Results are presented for three-dimensional flows over round and square cylinders and a realistic helicopter landing ship.

Youngs discusses Rayleigh–Taylor and Richtmyer–Meshkov mixing in Chapter 13. ILES is successfully applied to the three-dimensional simulation of Rayleigh–Taylor and Richtmyer–Meshkov mixing at high Reynolds number. The author argues that some form of monotonicity-preserving method is needed for these problems where there are density discontinuities and shocks. He shows how high-resolution ILES is currently making major contributions to understanding the Rayleigh–Taylor and Richtmyer–Meshkov mixing processes, constituting an essential tool for the construction and validation of engineering models for application to complex real applications.

Section D: Frontier flows

For the extremely complex flows of geophysics, astrophysics, and engineering discussed in this section, whole-domain scalable laboratory studies are impossible or very difficult. Deterministic simulation studies are very expensive and critically constrained by difficulties in (1) modeling and validating all the relevant physical subprocesses, and (2) acquiring all the necessary and relevant boundary condition information.

The section begins with a presentation by Smolarkiewicz and Margolin of ILES studies of geophysics in Chapter 14. The difficulties of modeling the dynamics of the global ocean and atmosphere (i.e., geostrophic turbulence) are compounded by the broad range of significant length scales (Re $\sim 10^8$) and by the relative smallness of the vertical height of these boundary layers in comparison with their horizontal extent, which accentuates the importance of the backscatter of energy to the larger scales of motion. In this chapter the authors demonstrate the ability of an ILES model based on high-order upwinding to reproduce the complex features of the global climate of the atmosphere and ocean.

Next, in Chapter 15, Porter and Woodward discuss their ILES-based studies of astrophysics. Homogeneous decaying and driven compressible turbulence (Re $\sim 10^{12}$), local area models of stellar convection, global models of red giant stars, and the Richtmyer–Meshkov mixing layer are examined in this context.

The section continues with Chapter 16, by Alin et al., on complex engineering turbulent flows, where they discuss the application of ILES to a variety of complex engineering-type applications ranging from incompressible external flows around typical naval applications to external and internal supersonic flows in aerospace applications. Cases examined include flows such as (1) the flow around a model scale submarine, (2) multi-swirl cumbustion flows, (3) solid rocket motor flows, and, (4) the flow and wave pattern around a modern surface combatant with transom stern.

Large-scale urban simulations are discussed by Patnaik et al. in Chapter 17. Airborne contaminant transport in cities presents challenging new requirements for computational fluid dynamics. The unsteady flow physics is complicated by very complex geometry, multiphase particle and droplet effects, radiation, latent and sensible heating effects, and buoyancy effects. Turbulence is one of the most important of these phenomena, and yet the overall problem is sufficiently difficult that the turbulence must be included efficiently with an absolute minimum of extra memory and computing time. This chapter describes a MILES methodology used as a simulation model for urban contaminant transport, and addresses the very difficult validation issues in this context.

Finally, outlook and open research issues are presented in Chapter 18.

SECTION A

MOTIVATION

1 More for LES: A Brief Historical Perspective of MILES

Jay P. Boris

1.1 Introduction to monotone integrated large eddy simulation

Turbulence is proving to be one of nature's most interesting and perplexing problems, challenging theorists, experimentalists, and computationalists equally. On the computational side, direct numerical simulation of idealized turbulence is used to challenge the world's largest computers, even before they are deemed ready for general use. The Earth Simulator, for example, has recently completed a Navier–Stokes solution of turbulence in a periodic box on a 4096 × 4096 × 4096 grid, achieving an effective Reynolds number somewhat in excess of 8000. Such a computation is impossible for nearly every person on the planet. Further, periodic geometry has little attraction for an engineer, and a Reynolds number of 8000 is far too small for most problems of practical importance.

The subject of this chapter is monotone integrated large eddy simulation (LES), or MILES – monotonicity-preserving implicit LES (ILES), a class of practical methods for simulating turbulent high-Reynolds-number flows with complicated, compressible physics and complex geometry. LES has always been the natural way to exploit the full range of computer power available for engineering fluid dynamics. When the dynamics of the energy-containing scales in a complex flow can be resolved, it is a mistake to average them out. Doing so limits the accuracy of the results, because uniform convergence to the physically correct answer, insofar as one exists, is automatically voided at the scale where the averaging has been performed. Even if the computational grid is refined repeatedly, the answer can get no better. At the same time, the overall resolution of a computation suffers when many computational degrees of freedom are expended unnecessarily on unresolved scales. Solving extra equations, for example, to define unresolved subgrid quantities is expensive and limiting.

Fortunately, we now know that a wide class of efficient fluid dynamics methods, generally based on monotone convection algorithms, has a built-in subgrid "turbulence" model that is coupled continuously to the grid-scale errors in the computed fluid dynamics. When the fluid dynamics embodies positivity-preserving or monotone (nonlinear) convection algorithms, the original name MILES applies. There are now hundreds of such algorithms and variations in use throughout the world. MILES works because the necessary physics, that is, conservation, monotonicity (positivity), causality, and locality, are built into the underlying fluid dynamics.

Professor John Lumley hosted a meeting at Cornell University in 1989, called Whither Turbulence: Turbulence at the Crossroads (Lumley 1990). The conference was focused on controversial questions in turbulence research that John felt had not been satisfactorily resolved. The program was structured as a dialog, with position papers on six major questions that were critiqued by several reviewers, reviewed, and subsequently published as a book. Professor W. C. Reynolds led the discussion of one of these questions with a keynote paper entitled “The Potential and Limitations of Direct and Large Eddy Simulations” (Reynolds 1990). This address summarized the situation in turbulence modeling at that time and was the jumping off point for my MILES paper. His exposition is highlighted in Section 1.2.

As a responding presenter, in my paper I focused on giving the evidence and reasons for the surpising success of monotone *no-model* LES methods. I named this approach to turbulence simulation *monotone integrated large eddy simulation*, or MILES, as an up-front reminder that monotone methods come with an integrated LES turbulence capability built in: “These monotone integrated LES algorithms are derived from the fundamental physical laws” (Boris 1990). The MILES hypothesis was formulated to explain “strong evidence suggesting that monotone convection algorithms (e.g., FCT), designed to satisfy the physical requirements of positivity and causality, in effect have a minimal LES filter and matching subgrid model already built in. The positivity and causality properties ... seem to be sufficient to ensure efficient transfer of the residual subgrid motions, as they are generated by resolved field mechanisms, off the resolved grid with minimal contamination of the well-resolved scales by the numerical filter.”

Looking back before the Cornell conference, my plunge into turbulence simulation actually dates to the early 1970s when flux-corrected transport (FCT) was invented. It soon became clear that FCT was good for much more than dynamic shocked flows, but recognizing just how much was going on under the surface in the computed solutions took almost another two decades, until 1989. Section 1.3 discusses the origins of FCT and the early “turbulence” computations performed with it. Section 1.4 extends this discussion to the properties of monotone methods that lend themselves to effective LES. Widespread acceptance that FCT and other monotone methods have a perfectly functional implicit subgrid turbulence model is taking as long again. This long delay is due in part to the fact that the result seems almost too good to be true. Even engineers and scientists with no previous LES persuasion have long been trained to decry the possibility of a free ride. Section 1.5 explains why it should not be surprising that MILES works well, and Section 1.6 considers some of the early tests performed to show how it was working.

Today, MILES’ growing acceptance is based in no small part on the work reported in the following chapters. With theoretical understanding and insight provided by the various authors, it is now easier to see why MILES works and to understand that there is a well-defined subgrid turbulence model in place. This chapter traces this evolving understanding, in a brief personal way. Here is a situation in which the complexity of the physical problem contributes to the ease of solution. Imitating the physics with the numerics, rather than cranking on a more formal mathematical approach, actually brings a big win. The MILES hypothesis evolved more as a growing realization than an invention. With 20:20 hindsight, perhaps it isn't surprising that it is taking others a long time to realize that this is one of those special cases where there can be a free ride.

1.2 The numerical simulation of turbulence

Turbulent flows are common in nature. They occur on space scales ranging from millimeters to megaparsecs. Such flows are extremely important for a number of reasons. Turbulence provides an efficient way for distinct, initially separate materials to interpenetrate and mix rapidly, and it provides for the rapid transport of heat and momentum to and from surfaces. In a typical turbulent flow, the important space and time scales can span many orders of magnitude, and these scales all coexist simultaneously in the same volume of fluid.

According to Reynolds (1990), the goals of LES are "to compute the three-dimensional, time-dependent details of the largest scales of motion (those responsible for the primary transport) using a simple model for the smaller scales. LES is intended to be useful in the study of turbulence physics at high Re, in the development of turbulence models, and for predicting flows of technical interest in demanding complex situations where simpler model approaches (e.g., Reynolds stress transport) are inadequate." The computational challenge is to resolve a wide enough range of scales to study the underlying physical mechanisms and provide a predictive capability for important practical applications.

Understanding LES is not possible without considering the Kolmogorov spectrum (Kolmogorov 1941, 1962). The kinetic energy density of turbulent motions is $\mathcal{E}(k)dk$ in the wave-number range from k to $k + dk$. This energy density, a function of the wave number, is expected to follow the power law

$$\mathcal{E}(k) = \mathcal{E}(1/L)(kL)^{-5/3}.$$

This Kolmogorov spectrum can be derived purely from dimensional arguments (Batchelor 1956) and describes how the energy density of turbulent structures of size $\eta = 1/k$ decreases rapidly with increasing wave number k. This relationship is generally valid only for an intermediate range of scales, called the *inertial range*, between the system size L and the small Kolmogorov scale, η_K, at which the viscous dissipation dominates the inertial flow of the fluid:

$$\eta_K = (\nu^3/\epsilon)^{1/4}.$$

This Kolmogorov scale is generally very small and may be micrometers, millimeters, or kilometers where the system length is of the order of meters, kilometers, or parsecs.

The turbulence energy density $\mathcal{E}(k)$ decreases with increasing k. It results from a process in which the dynamic structures in the fluid (called *eddies*) of size $1/k$ interact