2 A Rationale for Implicit LES

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2.1 Introduction

High-Reynolds' number turbulent flows contain a broad range of scales of length and time. The largest length scales are related to the problem geometry and associated boundary conditions, whereas it is principally at the smallest length scales that energy is dissipated by molecular viscosity. Simulations that capture all the relevant length scales of motion through numerical solution of the Navier–Stokes equations (NSE) are termed *direct numerical simulation* (DNS). DNS is prohibitively expensive, now and for the foreseeable future, for most practical flows of moderate to high Reynolds' numbers. Such flows then require alternate strategies that reduce the computational effort. One such strategy is the Reynolds-averaged Navier–Stokes (RANS) approach, which solves equations averaged over time, over spatially homogeneous directions, or across an ensemble of equivalent flows. The RANS approach has been successfully employed for a variety of flows of industrial complexity. However, RANS has known deficiencies when applied to flows with significant unsteadiness or strong vortex-acoustic couplings.

Large eddy simulation (LES) is an effective approach that is intermediate in computational complexity while addressing some of the shortcomings of RANS at a reasonable cost. An introduction to conventional LES is given in Chapter 3. The main assumptions of LES are (1) that the transport of momentum, energy, and passive scalars is mostly governed by the unsteady features in the larger length scales, which can be resolved in space and time; and (2) that the smaller length scales are more universal in their behavior so that their effect on the large scales (e.g., in dissipating energy) can be represented by using suitable subgrid-scale (SGS) models. Many different approaches have been developed for the construction of SGS models; some of these are described in Chapter 3. It is essential to recognize that in the absence of a universal theory of turbulence, the construction of SGS models is unavoidably pragmatic, based primarily on the rational use of empirical information.

We distinguish between two general classes of SGS models. Simple *functional* SGS models focus on dissipating energy at a physically correct rate and are based on an artificial "eddy" viscosity. More sophisticated and accurate *structural* models attempt to address issues of the transfer of energy between length scales, and are based on a variety of ideas such as scale similarity and approximate deconvolution. The latter models typically do not dissipate sufficient energy to ensure computational stability, which has led to the development of mixed models that combine the positive features of the two classes of models. The results of such mixed models have been more satisfactory, but the complexity of their implementation and the computational effort required to employ them have limited their popularity. This situation has motivated the investigation of unconventional LES approaches, such as implicit LES (ILES) – the subject of this volume, adaptive flux reconstruction (e.g., Adams 2001), and variational schemes with embedded subgrid stabilization (e.g., Hughes 1995). The underlying idea of these new approaches is to represent the effects of the unresolved dynamics by regularizing the larger scales of the flow. Such regularization may be based on physical reasoning resulting from an ab initio scale separation, or on numerical constraints that enforce the preservation of monotonicity or, more generally, ensure nonoscillatory solutions. Enforcing such numerical constraints is the common thread that relates the various nonoscillatory finite-volume (NFV) numerical methods employed in ILES. The absence of explicit SGS models in the ILES approach offers many practical advantages, both of computational efficiency and ease of implementation. However, these alone are not sufficient reasons to justify ILES. At a more fundamental level, it is essential to understand why and how well this approach works in practical circumstances, while simultaneously recognizing its limits of applicability. One might argue that the more conventional LES approaches should be similarly scrutinized, though in general this is not systematically done. Nevertheless, in this chapter we will attempt to justify the ILES approach. Our basic thesis is this: *ILES works because it solves the equations that most accurately represent the dynamics of finite volumes of fluid – i.e., governing the behavior of measurable physical quantities on the computational cells.*

In general, there are approximation errors in numerical simulations even for the resolved scales of motion. One can identify the errors of a numerical algorithm by using modified equation analysis (MEA; see Chapter 5); these errors take the form of truncation terms that augment the analytic equations. It has been pointed out by Hirt (1969) and more recently by Ghosal (1996) that, in typical flow regimes, these truncation terms have the same order of magnitude as the SGS terms in LES. The purpose of those observations was to emphasize the importance of controlling the truncation errors; that is, a well-resolved LES requires accurate discretizations and adequate computational grids. However, one might naturally ask whether one could design the numerical algorithms so that the truncation terms would themselves serve as SGS models.

Why should the governing equations for numerical simulation be different from the continuum partial differential equations (PDEs)? The PDEs such as NSE that govern fluid motion are first derived in integral form by using the conservation principles of physics. The well-known PDE forms are then recovered in the limit that the integration volume shrinks to a point. The operable question then is this: What form do the equations take for finite values of the integration volume such as a computational cell? From the point of view of consistency, one would expect that the governing equations for these finite volumes would be the PDEs, augmented by additional terms that depend on the size of the volume. We will refer to these governing equations as *finite-volume equations*, and the additional terms as *finite-volume corrections*. We note that, most generally, the volume will include both space and time scales.

We begin in the next section by providing a historical perspective of ILES. We then continue by describing other theories, both analytic and numerical, that address the form of these finite-volume corrections. We shall find that all of these treatments lead to remarkably similar corrections; when a finite-volume momentum equation is derived, it contains new terms that are a nonlinear combination of first and second spatial derivatives with a dimensional coefficient that depends on the volume of integration. In addition, we recount the connection between the SGS models and NFV numerical methods, which have a common origin in the artificial viscosity of von Neumann and Richtmyer.

In Section 2.3, we will present a derivation of the finite volume equation for two-dimensional incompressible Navier–Stokes flows. The derivation closely follows the format described in Margolin and Rider (2002) for the one-dimensional Burgers' equation. However, the multidimensionality of the calculation brings out a new feature of the finite-volume equations, namely that their tensor properties depend on the details of the shape, as well as the magnitude, of volume of integration.

In Section 2.4, we exhibit the MEA derived from the approximation of the 2D NSE obtained with a particular class of NFV algorithms, known as MPDATA (see Chapter 4d). We will discuss the similarities to the finite-volume 2D NSE as well as the differences. In Section 2.5, we delve more deeply into the energy equations associated with both the finite-volume and the MPDATA approximate of 2D NSE. The purpose of these sections is to lay the groundwork for Chapter 5, where we will identify the features of a numerical method required for ILES and where we will compare the strengths and weaknesses of individual NFV methods on which ILES is based, in terms of their inherent dissipative properties.

2.2 Historical perspective

In their 1993 paper, Oran and Boris (1993) noted a "convenient conspiracy" in the numerical simulation of certain complex flows, wherein a physical model can combine with the numerical method to produce excellent results. Beyond the scope of their original discussion, the important point to note here is that the class of physical models that they considered – e.g., Burgers' equation, and the compressible and incompressible versions of NSEs – have the common feature of a quadratic nonlinearity in the advective terms. Further, on the numerical side, the advective terms discussed by Oran and Boris were formulated with monotonicity-preserving approximations. We will see in the next section that a MEA of such approximations leads to a dissipation of kinetic energy proportional to the cube of the velocity gradients. This is similar to theoretical results that are described below.

To better understand the connection of physical theory and numerical discretizations, it is useful to begin by describing the role of dissipation in ensuring numerical stability. In order for a numerical method to be stable, it must be dissipative in the sense of the energy or the L_2 norm. However, stability is not sufficient to guarantee physically realizable solutions. To ensure unique, physically meaningful solutions, a finite amount of dissipation must be present at a minimum. *This finite dissipation is referred to as an entropy condition. In principle, this dissipation may be implemented as part of the physical model (i.e., explicitly) or as part of the numerical method (i.e., implicitly).*

Historically, numerical dissipation was found to be necessary and was implemented in Lagrangian simulations of high-speed flows with shocks, where the equations were explicitly augmented by dissipative terms known as *artificial viscosity* (Richtmyer 1948; von Neumann and Richtmyer 1950). As we shall recount shortly, this idea was extended to turbulent flows, where the dissipative terms became known as SGS models. The development of explicit SGS models for turbulence has continued and grown ever more sophisticated. However, the evolution of artificial viscosity took a different turn in the early 1970s, when Jay Boris and Bram van Leer independently introduced the first nonoscillatory methods. In these methods, the entropy condition is satisfied implicitly as part of the numerical method. Over the past 30 years, many new improved nonoscillatory methods have been developed.

Nonoscillatory methods for shock flows exhibit many advantages over other approaches, including nonlinear stability, computational efficiency, ease of implementation, and, above all, accurate and realistic results. Examples of these methods used in ILES will be described in Chapter 4. For these reasons, such methods have become the preferred choice for many problems in the field of computational fluid mechanics. It would seem compelling, then, that this implicit approach should be investigated for turbulent flows. This is, in fact, ILES – the subject of this volume.

While it may not be possible to sort out the earliest efforts at simulating turbulent flows with NFV schemes, it is clear that credit for the first public documentation of the approach belongs to Jay Boris and colleagues at the U.S. Naval Research Laboratory (Chapters 1 and 8). Boris made the crucial early connection (Boris 1990), namely that the truncation errors of such algorithms could in fact serve as a SGS model in what he denoted the Monotone Integrated LES (MILES) approach. Further, he recognized that this was not a special feature of the flux-corrected transport (FCT) algorithm (Chapter 4a) on which he based MILES, but that this implicit property *could apply equally for a number of other suitably formulated monotone methods as well.* MILES applications using monotonic algorithms coupled to various physical processes in shear-flow engineering applications are extensively reviewed in this volume (Chapters 8–11, 16, and 17). The ILES work of Woodward and colleagues with the piecewise parabolic method (Chapter 4b) involved studies of homogeneous turbulence in the early 1990s (Chapter 7) and astrophysical problems in regimes of highly compressible flow with extremely high Reynolds' numbers (Chapter 15). At about the same time, David Youngs and colleagues applied van Leer methods (Chapter 4c) to modeling the growth of turbulent regions and the mixing resulting from fluid instabilities, including Raleigh–Taylor, Kevin–Helmholtz, and Richtmyer–Meshkov (Chapter 13). These applications involve adjacent regions of very high and very low Reynolds' number, illustrating a very useful feature of ILES – that the same fluid solver can be used for smooth and for turbulent flows. The vorticity confinement method (Chapter 4e) introduced by Steinhoff, also in the early 1990s, invoked ideas similar to those in shock capturing. This is an approach to ILES based directly on the discrete equations satisfied within thin, modeled vortical regions; this approach is especially well suited to treat engineering flows over blunt bodies, including attached and separating boundary layers, and resulting turbulent wakes (Chapter 12). Margolin, Smolarkiewicz, and colleagues published the first applications of ILES to geophysics using MPDATA (Chapters 4d and 14). As in the astrophysics cases, the geophysical calculations typically involve very high Reynolds' numbers ($\text{Re} \sim 10^6$), but with stratified and nearly incompressible flow.

The effectiveness of the ILES approach demonstrated in a wide range of applications in engineering, astrophysics, and geophysics does not address the question of why the approach is successful. A significant contribution was made by Fureby and Grinstein (1999, 2002), regarding the similarity between certain NFV schemes and the explicit SGS models used in conventional LES. These authors used the MEA framework to show that a particular class of flux-limiting algorithms (Chapter 4a) with dissipative leading-order terms provide appropriate built-in (implicit) SGS models of a mixed tensorial (generalized) eddy-viscosity type. Key features in the comparisons with classical LES leading to the identification of this implicit SGS model were the MEA framework and the finite-volume formulation (also used in this chapter), which readily allowed the recasting of the leading-order truncation terms in divergence form. A similar direction was also explored by Rider and Margolin (2003), who compared the implicit SGS models resulting from a MEA of several NFV algorithms in one dimension and showed the connections to explicit SGS models. A systematic MEA of ILES is further presented in Chapter 5.

The intuitive basis for the pioneering ILES work of Boris, Woodward, Youngs, Steinhoff, and their collaborators was most largely formed as a natural follow-up to shock-capturing methods. However, a more rigorous physical basis for ILES suggested by Margolin and Rider (2002) arose from examining the correspondence of the entropy conditions themselves, as derived in various theories compared with the MEA of nonoscillatory methods. Our next step, then, is to list some of these fundamental theoretical results.

Frisch (1995) derived a formula for the dissipation of energy in a Burgers' fluid arising solely at the shock wave:

$$\left\langle \frac{\partial K}{\partial t} \right\rangle \ell = \frac{1}{12} \langle \Delta u \rangle^3, \tag{2.1}$$

where K is the kinetic energy, and angle brackets indicate spatial averaging over the length ℓ.

Bethe (1942) showed that the rate of entropy production across a shock is

$$T\frac{\partial S}{\partial t} = -\frac{\mathcal{G}}{12c_s}\langle \Delta u \rangle^3, \tag{2.2}$$

where S is the entropy, T is the temperature, c_s is the sound speed, and $\mathcal{G}$ is the fundamental thermodynamic derivative

$$\mathcal{G} \equiv \frac{\partial^2 P}{\partial V^2}. \tag{2.3}$$

Kolmogorov (1962) derived a remarkably similar form for the inviscid dissipation of kinetic energy in isotropic incompressible turbulence:

$$\left\langle \frac{\partial K}{\partial t} \right\rangle \ell = -\frac{\partial S}{\partial t}\ell = \frac{5}{4}\langle \Delta u \rangle^3. \tag{2.4}$$

This similarity of the forms of energy dissipation, or entropy creation, was noted by Margolin and Rider (2002), who pointed out that each case combines the features of *inviscid* dissipation of kinetic energy with finite scales of observation. Further, these theoretical results show a connection between the large-scale behavior of shocked flows and of turbulence. The authors also noted the similarity of these forms to the classic artificial viscosity of von Neumann and Richtmyer (1950), which is used to ensure sufficient entropy production in numerical simulations of shocks. They went on to recount the historic connection of artificial viscosity and the early SGS turbulence models of Smagorinsky, which is reproduced here. Smagorinsky's generalization of artificial viscosity employs a scalar (i.e., isotropic) diffusivity. However, it is now well established that the near-dissipation end region of the inertial subrange is inherently anisotropic and characterized by very thin filaments (worms) of intense vorticity with largely irrelevant internal structure, embedded in a background of weak vorticity (e.g., Jimenez et al. 1993). As previously noted by Fureby and Grinstein (1999, 2002), the implicit SGS models associated with NFV methods naturally contain a tensor diffusivity that is able to regularize the unresolved scales without losing essential directional information, while their ability to capture steep gradients can be used to emulate (near the ILES cutoff) the dissipative features of the *high end* of the physical inertial subrange region. In Section 2.4, we will exhibit the tensor diffusivity of a particular NFV scheme to illustrate this point (see also Chapters 4a and 5).

In the rest of this section, we will expand on the connection between numerical simulations of shock flows and turbulence and extend the discussion to include nonoscillatory numerical methods. Indeed, the developments of NFV methods and SGS models for turbulent flow both stem from the earlier concept of artificial viscosity for the computation of shock waves on a finite grid. This viscosity is constructed to mimic the physical production of entropy across a shock – such as shown in Eq. (2.2) – without resolving the viscous processes that are responsible, and to reproduce the correct jump conditions. The strategy is often referred to as *shock capturing* or *regularization*. One important and noticeable result of artificial viscosity is the suppression of Gibbs phenomena (unphysical oscillations) associated with the discrete jump. Further, the artificial viscosity guarantees the nonlinear stability of the simulation (under a proper time-step limit).

Artificial viscosity was conceived for Lagrangian simulations of shocks; however, Eulerian simulations of shocks and also of turbulence also exhibit unphysical oscillations, and it is not difficult to imagine that one might try to extend the concept to these simulations as well. The connection to turbulent flows and SGS models appeared first, at the very dawn of numerical weather and climate prediction.

After World War II, John von Neumann worked to expand the role of simulation in science. One of his efforts was in the area of numerical weather prediction, where he worked with Jules Charney at the Institute for Advanced Study during the early 1950s. In 1956, von Neumann and Charney were present at a conference where Norman Phillips presented his two-dimensional simulation of a month of weather of the Eastern North America area. Also present was a graduate student, Joseph Smagorinsky. It was observed that Phillip's calculation was polluted by ringing late in the simulated month, and Charney made the suggestion that von Neumann's viscosity could be used to eliminate that ringing. Smagorinsky was given the task of extending Phillip's results to three dimensions, including artificial viscosity.

Smagorinsky's implementation (Smagorinsky 1963, 1983) resulted in the first SGS model, and it formed the basis for much future work. After the fact, a more rigorous connection of the Smagorinsky eddy viscosity to turbulence theory was made by Lilly (1966). SGS modeling has since grown and evolved. However, the energy dissipation associated with the original Smagorinsky form persists in many more sophisticated models such as the popular dynamic Smagorinsky models and mixed models.

The path to nonoscillatory methods was a little less direct, and began with the early work of Peter Lax (Lax 1954, 1972). In particular, a paper by Lax and Wendroff (1960) first emphasized the importance of conservative methods (cf. finite-volume methods; flux methods). A later paper (Lax and Wendroff 1964) described a second-order-accurate numerical approximation for the advective terms in which first-order diffusive errors are directly compensated. That Lax–Wendroff scheme produces oscillatory fields behind a shock wave, in contrast to the Lax–Friedrichs method, which produces monotone shock transitions but is overly diffusive.* Both methods differ in an essential way from the artificial viscosity methods in that they are "linear." Specifically, a linear method uses the same stencil everywhere, whereas artificial viscosity is nonlinear in the sense that its magnitude depends on the flow variables. However, it took almost 20 more years for the importance of nonlinearity to be recognized.

Sergei Godunov was a graduate student in the Soviet Union in the early 1950s. As part of his doctoral thesis, he was assigned to calculate shock-wave propagation. At the time, existing algorithms in the Soviet Union were not sufficiently accurate, and

* Lax–Wendroff methods usually employ an artificial viscosity to control oscillations behind shocks.

Godunov was not familiar with the work of Lax and Friedrichs (not easily available to him because of the Cold War; see Godunov 1999). Instead, he developed a new methodology, based on solving local Riemann problems, that not only satisfied his degree requirements but sowed the seeds of a computational revolution 20 years later. Perhaps of equal importance, Godunov proved a fundamental theorem, which states that no numerical method can be simultaneously linear, second-order accurate, and monotonicity preserving (see, e.g., LeVeque 1999).

Godunov's method and theorem were published in 1959 (the manuscript was completed in 1956). However, it was largely ignored and lay dormant for over a decade. Then in 1971, two scientists, Jay Boris in the United States and Bram van Leer in the Netherlands, overcame the barrier of Godunov's theorem by recognizing the feasibility of giving up linearity. The FCT method (Boris and Book 1973) focused on eliminating unphysical oscillations. It is a hybrid scheme that mixes first-order and second-order accuracy in a nonlinear manner. The MUSCL schemes of van Leer (1979) are a more direct generalization of Godunov's method in which the initial states of the underlying Riemann problem are modified by limiting the magnitude of gradients.

(Aside: As fate would have it, a third scientist, Kolgan, produced an alternate generalization of Godunov's method that also overcame the barrier of Godunov's theorem. In today's parlance, his method would take the label of a second-order essentially nonoscillatory, or ENO, method. Unfortunately, this work went unnoticed and Kolgan died before receiving any recognition.)

By the 1980s, the nonoscillatory approach was widely accepted and produced a plethora of ideas and implementations. Some of these are described in more detail in Chapter 4 of this volume. Many more may be expected to work for ILES, but perhaps not all. In Section 2.4 of this chapter and later in Chapter 5, we will investigate the requirements for successful ILES in more detail.

To summarize this section, sufficient dissipation to satisfy entropy conditions is necessary to achieve physically realizable simulations. The entropy conditions can be seen to be dependent on the mesh resolution, based on the successful form of artificial viscosity and more simply on dimensional analysis. This is consistent with our observation in the previous section, that the governing equations for volume-averaged quantities should depend on the size of the volume elements. Furthermore, we note that it is the nonlinearity of the advective terms that gives rise to these extra terms, and that it is the use of nonlinear approximations that allows the formulation of ILES methods. In the next section, we will explore these ideas in more mathematical detail.

2.3 A Physical perspective

In this section, we derive the finite-volume equation for the 2D incompressible NSE. Our derivation generally follows that in Margolin and Rider (2002), which was applied to the 1D Burgers' equation; however, we will ignore the averaging in time here. First, we will consider the case of smooth (laminar) flow. Then we will show that the same results apply to turbulent flow.

2.3.1 Laminar flows

The Navier–Stokes equations for the two-component velocity vector, $U = (u, v)$, are

$$\frac{\partial u}{\partial t} = -(u\,u)_x - (u\,v)_y - P_x + \nu\,(u_{xx} + u_{yy}),$$
$$\frac{\partial v}{\partial t} = -(u\,v)_x - (v\,v)_y - P_y + \nu\,(v_{xx} + v_{yy}), \tag{2.5}$$

plus the equation of incompressibility

$$u_x + v_y = 0, \tag{2.6}$$

where the shorthand notation, $u_x \equiv \frac{\partial u}{\partial x}$, is used for spatial differentiation. Here, P is the pressure and ν is the coefficient of physical viscosity. We note that the pressure is a diagnostic variable and can be found by solving an elliptic equation that enforces incompressibility.

We define volume-averaged velocities

$$\bar{u}(x, y) \equiv \frac{1}{\Delta x\, \Delta y} \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} u(x', y')\, dx'\, dy' \tag{2.7}$$

and

$$\bar{v}(x, y) \equiv \frac{1}{\Delta x\, \Delta y} \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} v(x', y')\, dx'\, dy'. \tag{2.8}$$

That is, here we have chosen the volume of integration to be a rectangle, mimicking a computational cell in a regular mesh.

Our goal is to find evolution equations for $\bar{U} = (\bar{u}, \bar{v})$. To begin, we note that (2.6) is linear. Hence the spatial differentiation and the volume averaging commute, and it immediately follows that

$$\bar{u}_x + \bar{v}_y = 0. \tag{2.9}$$

Similar arguments apply to the time derivatives and the viscous terms in (2.5). However, the nonlinearity of the advective terms requires more care. Here we will generalize the calculation of Margolin and Rider (2002) to two dimensions. To evaluate terms such as

$$\mathcal{I}_1 = \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} u\, u_x\, dx'\, dy',$$

the basic idea is to expand the integrand in a Taylor series. For this series to converge, the velocity field has to be smooth on the length scales Δx and Δy. This is true for low-Reynolds' number flows, which are amenable to DNS. It is unlikely to be true for flows that we consider for LES, where the Reynolds' number is large and the dissipative scales are not resolved on the mesh. In this subsection, we will consider the case of smooth flows and indicate the steps to evaluate integrals like $\mathcal{I}_1$. In the next section, we will show how one can extend these results to LES regimes.

We begin by assuming that the velocity field can be expanded in a convergent Taylor series on the scales Δx and Δy:

$$
\begin{aligned}
u(x+x', y+y') &\approx u(x,y) + u_x\, x' + u_y\, y' + u_{xx}\frac{(x')^2}{2} \\
&\quad + u_{xy}\, x'y' + u_{yy}\frac{(y')^2}{2} + \text{HOT}, \\
v(x+x', y+y') &\approx v(x,y) + v_x\, x' + v_y\, y' + v_{xx}\frac{(x')^2}{2} \\
&\quad + v_{xy}\, x'y' + v_{yy}\frac{(y')^2}{2} + \text{HOT},
\end{aligned}
\tag{2.10}
$$

where HOT indicates terms of higher order. Substituting these expansions into definitions (2.7) and (2.8) immediately yields

$$
\bar{u}(x,y) \approx u(x,y) + \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 u_{xx} + \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 u_{yy} + \text{HOT} \tag{2.11}
$$

and

$$
\bar{v}(x,y) \approx v(x,y) + \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 v_{xx} + \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 u_{yy} + \text{HOT}. \tag{2.12}
$$

These volume-averaged velocities are continuous functions of space and time. Note that, by symmetry, the averaged functions are even in Δx and Δy. Now the higher-order derivatives like $\bar{u}_x$ can be derived by differentiating (2.11) and (2.12). For example,

$$
\bar{u}_x \approx u(x,y) + \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 u_{xxx} + \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 u_{xyy} + \text{HOT}. \tag{2.13}
$$

We will have the need for the inverse relations corresponding to (2.11) and (2.12). These are easily found to be

$$
u(x,y) \approx \bar{u} - \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 \bar{u}_{xx} - \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 \bar{u}_{yy} + \text{HOT} \tag{2.14}
$$

and

$$
v(x,y) \approx \bar{v} - \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 \bar{v}_{xx} - \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 \bar{v}_{yy} + \text{HOT}. \tag{2.15}
$$

There are four quadratic terms to evaluate:

$$
\begin{aligned}
\mathcal{I}_1 &= \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} 2\,u\,u_x\,dx'\,dy', \\
\mathcal{I}_2 &= \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} \left(v\,u_y + v_y\,u\right) dx'\,dy', \\
\mathcal{I}_3 &= \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} \left(u\,v_x + u_x\,v\right) dx'\,dy', \\
\mathcal{I}_4 &= \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \int_{y-\frac{\Delta y}{2}}^{y+\frac{\Delta y}{2}} 2\,v\,v_y\,dx'\,dy'.
\end{aligned}
\tag{2.16}
$$

The general strategy to evaluate each of these terms is to insert the Taylor expansions into the integrand and multiply. We note that only terms that are even in the integration variables x' and y' will contribute. Then

$$
\begin{aligned}
\mathcal{I}_1 = 2uu_x &+ \frac{3\,u_x\,u_{xx} + u\,u_{xxx}}{\Delta x\,\Delta y} \int_{-1/2\Delta x}^{1/2\Delta x} \int_{-1/2\Delta y}^{1/2\Delta y} (x')^2\,dx'\,dy' \\
&+ \frac{2\,u_y\,u_{xy} + u\,u_{xyy} + u_x\,u_{yy}}{\Delta x\,\Delta y} \int_{-1/2\Delta x}^{1/2\Delta x} \int_{-1/2\Delta y}^{1/2\Delta y} (y')^2\,dx'\,dy'.
\end{aligned}
\tag{2.17}
$$

Evaluating the integrals leads to

$$
\mathcal{I}_1 = 2uu_x + \frac{1}{3}\left(\frac{\Delta x}{2}\right)^2 (3u_xu_{xx} + uu_{xxx}) + \frac{1}{3}\left(\frac{\Delta y}{2}\right)^2 (2u_yu_{xy} + u_xu_{yy} + uu_{xyy}).
\tag{2.18}
$$

Equation (2.18) is not yet in useful form, since $\mathcal{I}_1$ is written in terms of u rather than $\bar{u}$. We can rewrite the equation in the desired form by using the inverse relations (2.14) and (2.15). This approach is similar to approximate deconvolution described in more detail in Chapter 6. For example,

$$
\begin{aligned}
uu_x &\approx \left[\bar{u} - \left(\frac{\Delta x^2}{24}\right)\bar{u}_{xx} - \left(\frac{\Delta y^2}{24}\right)\bar{u}_{yy}\right]\left[\bar{u}_x - \left(\frac{\Delta x^2}{24}\right)\bar{u}_{xxx} - \left(\frac{\Delta y^2}{24}\right)\bar{u}_{xyy}\right] \\
&\approx \bar{u}\bar{u}_x - \left(\frac{\Delta x^2}{24}\right)(\bar{u}_x\bar{u}_{xx} + \bar{u}\bar{u}_{xxx}) - \left(\frac{\Delta y^2}{24}\right)(\bar{u}_x\bar{u}_{yy} + \bar{u}\bar{u}_{xyy}).
\end{aligned}
\tag{2.19}
$$

Putting all the terms together, the result for $\mathcal{I}_1$ is

$$
\begin{aligned}
\mathcal{I}_1 &= 2\bar{u}\bar{u}_x + \frac{2}{3}\left(\frac{\Delta x}{2}\right)^2 \bar{u}_x\bar{u}_{xx} + \frac{2}{3}\left(\frac{\Delta y}{2}\right)^2 \bar{u}_y\bar{u}_{xy} \\
&= (\bar{u}^2)_x + \frac{1}{3}\left(\frac{\Delta x}{2}\right)^2 \left[(\bar{u}_x)^2\right]_x + \frac{1}{3}\left(\frac{\Delta y}{2}\right)^2 \left[(\bar{u}_y)^2\right]_x.
\end{aligned}
\tag{2.20}
$$

The same procedure can be applied for $\mathcal{I}_2$, $\mathcal{I}_3$, and $\mathcal{I}_4$. The final result for the volume-averaged momentum equations is, to $\mathcal{O}(\Delta x^2, \Delta y^2)$,

$$\begin{aligned}\frac{\partial \bar{u}}{\partial t} =& - (\bar{u}^2)_x - (\bar{v}\bar{u})_y - \frac{1}{3}\left(\frac{\Delta x}{2}\right)^2 \left[(\bar{u}_x\bar{u}_x)_x + (\bar{v}_x\bar{u}_x)_y\right] \\ &- \frac{1}{3}\left(\frac{\Delta y}{2}\right)^2 \left[(\bar{u}_y\bar{u}_y)_x + (\bar{u}_y\bar{v}_y)_y\right] - \bar{P}_x + \nu(\bar{u}_{xx} + \bar{u}_{yy}), \end{aligned} \tag{2.21}$$

$$\begin{aligned}\frac{\partial \bar{v}}{\partial t} =& - (\bar{u}\bar{v})_x - (\bar{v}^2)_y - \frac{1}{3}\left(\frac{\Delta x}{2}\right)^2 \left[(\bar{u}_x\bar{v}_x)_x + (\bar{v}_x\bar{v}_x)_y)\right] \\ &- \frac{1}{3}\left(\frac{\Delta y}{2}\right)^2 \left[(\bar{u}_y\bar{v}_y)_x + (\bar{v}_y\bar{v}_y)_y\right] - \bar{P}_y + \nu(\bar{v}_{xx} + \bar{v}_{yy}). \end{aligned} \tag{2.22}$$

We emphasize that this result is specific for the rectangular volume of integration.

2.3.2 Renormalization

When the velocity field is not smooth on the scales of the integration volume, its truncated Taylor series is not an accurate approximation throughout the volume and the derivation of the previous section is not justifiable. In this section, we will consider a more general approach that extends our results to high-Reynolds' number flows. Remarkably, we will find that the results of the previous section remain valid, indicating the renormalizability of the averaging of the advective terms.

The fact that the averaging process is also a smoothing process leads naturally to a new question: Will the averaged velocity always be "smooth enough" on the scale of the averaging? We will simply assume this to be true, seeing it as a necessary prerequisite to practical computer simulation of turbulence. More precisely, let us assume that the finite-scale equations, (2.21) and (2.22), are valid on the length scales Δx and Δy. We will show that this implies their validity on the scales $2\Delta x$ and $2\Delta y$. Since we know these equations are valid on some scales, such as in the DNS range, we can use induction to conclude that the finite-scale equations derived in the previous section are valid at all scales. This implies that the entropy condition is ensured through this process.

Let us consider a rectangle $2\Delta x$ by $2\Delta y$. This can be thought of as four Δx by Δy rectangles. A volume-averaged velocity $\bar{U} = (\bar{u}, \bar{v})$ is defined at the center of each of these smaller rectangles. Because the integrals that define $\bar{U}$ are simply additive – see (2.7) – we can define the volume average over the larger rectangle:

$$\begin{aligned}\widehat{u}(x, y) &= \frac{1}{4\Delta x\Delta y}\int_{-\Delta x}^{\Delta x}\int_{-\Delta y}^{\Delta y} u(x + x', y + y')\,dx'\,dy' \\ &= \frac{1}{4}\left[\bar{u}(+, +) + \bar{u}(+, -) + \bar{u}(-, -) + \bar{u}(-, +)\right], \end{aligned} \tag{2.23}$$

where for brevity we have written $\bar{u}(+,+) \equiv \bar{u}\left(x+\frac{\Delta x}{2}, y+\frac{\Delta y}{2}\right)$. Taylor expanding the four terms inside the brackets in this equation leads (to second order) to

$$\widehat{u} = \bar{u} + 1/2\bar{u}_{xx}\left(\frac{\Delta x}{2}\right)^2 + 1/2\bar{u}_{yy}\left(\frac{\Delta y}{2}\right)^2, \tag{2.24}$$

where now all functions are centered at coordinates (x, y). This implies the inverse relation,

$$\bar{u} = \widehat{u} - 1/2\widehat{u}_{xx}\left(\frac{\Delta x}{2}\right)^2 - 1/2\widehat{u}_{yy}\left(\frac{\Delta y}{2}\right)^2. \tag{2.25}$$

Now let us calculate

$$\begin{aligned}\widehat{\mathcal{I}}_1 &= \frac{1}{4\Delta x \Delta y}\int_{-\Delta x}^{\Delta x}\int_{-\Delta y}^{\Delta y} 2uu_x dx'\, dy' \\ &= \frac{1}{4}\left[\mathcal{I}(+,+)_1 + \mathcal{I}(+,-)_+\mathcal{I}(-,-)_1 + \mathcal{I}(-,+)_1\right].\end{aligned} \tag{2.26}$$

From the symmetry of (2.26), it is clear that linear terms in Δx and Δy will cancel, and the quadratic terms are identical for all four terms. So it is sufficient to consider $\mathcal{I}(+,+)$, keeping only the even terms. Then

$$\begin{aligned}\bar{u}(+,+) &= \bar{u} + \bar{u}_x\frac{\Delta x}{2} + \bar{u}_y\frac{\Delta y}{2} + u_{xx}\frac{\Delta x^2}{4} + u_{yy}\frac{\Delta y^2}{4}\cdots \\ \bar{u}_x(+,+) &= \bar{u}_{xx} + \bar{u}_{xx}\frac{\Delta x}{2} + \bar{u}_{xy}\frac{\Delta y}{2} + u_{xxx}\frac{\Delta x^2}{4} + u_{xyy}\frac{\Delta y^2}{4}\cdots\end{aligned} \tag{2.27}$$

and

$$\begin{aligned}\widehat{\mathcal{I}}_1 =& 2\bar{u}\bar{u}_x + 2\left(\frac{\Delta x}{2}\right)^2\left[\frac{11}{6}\bar{u}_x\bar{u}_{xx} + 1/2\bar{u}\bar{u}_{xxx}\right] \\ &+ 2\left(\frac{\Delta y}{2}\right)^2\left[\frac{8}{6}\bar{u}_y\bar{u}_{xy} + 1/2\bar{u}\bar{u}_{xyy} + 1/2\bar{u}_x\bar{u}_{yy}\right].\end{aligned} \tag{2.28}$$

Finally, we use the inverse relations, (2.25), to rewrite this expression in terms of $\widehat{u}$:

$$2\bar{u}\bar{u}_x = 2\widehat{u}\widehat{u}_x - \left(\frac{\Delta x}{2}\right)^2[\widehat{u}_x\widehat{u}_{xx} + \widehat{u}\widehat{u}_{xxx}] - \left(\frac{\Delta y}{2}\right)^2[\widehat{u}_x\widehat{u}_{yy} + \widehat{u}\widehat{u}_{xyy}],$$

leading to

$$\begin{aligned}\widehat{\mathcal{I}}_1 &= 2\widehat{u}\widehat{u}_x + \frac{2\Delta x^2}{3}\widehat{u}_x\widehat{u}_{xx} + \frac{2\Delta y^2}{3}\Delta y^2\widehat{u}_y\widehat{u}_{xy} \\ &= (\widehat{u}^2)_x + \frac{\Delta x^2}{3}\left[(\widehat{u}_x)^2\right]_x + \frac{\Delta y^2}{3}\left[(\widehat{u}_y)^2\right]_x.\end{aligned} \tag{2.29}$$

That is, we have reproduced (2.20) when the averaging volume now is $2\Delta x$ by $2\Delta y$. The same calculation is readily repeated for $\mathcal{I}_2$, $\mathcal{I}_3$, and $\mathcal{I}_4$, and each of these terms is unchanged except for the doubling of the length scales. Thus, we conclude that the finite-scale equations, (2.21) and (2.22), are valid for all averaging volumes, whether the Reynolds' number associated with those scales is small (DNS) or large (LES).

2.3.3 Discussion of the finite-scale equations

Here, we will make several observations about the finite-scale equations, (2.21) and (2.22). First, we repeat that the derivation is a straightforward extension of that in Margolin and Rider (2002), and that there is no obstacle to further extending the results to three spatial dimensions and to include time averaging as well.

Second, we note that the lowest-order finite-scale corrections are quadratic in the mesh spacings Δx and Δy (at lowest order) and that there are no terms of order $\Delta x\ \Delta y$. The result does depend on both the size and shape of the volume chosen for averaging. We have chosen rectangles in two dimensions to emphasize the comparisons with our numerical results in the next two sections.

Third, we note that the finite-scale corrections have the form of the divergence of a symmetric tensor, which implies the conservation of the finite-scale momentum. In the language of LES, the finite-scale corrections correspond to the divergence of a SGS tensor, $\nabla \cdot \tau$, where

$$\tau^{xx} = -\frac{1}{3}\left[\left(\frac{\Delta x}{2}\right)^2 \bar{u}_x^2 + \left(\frac{\Delta y}{2}\right)^2 \bar{u}_y^2\right] \tag{2.30}$$

$$\tau^{xy} = \tau^{yx} = -\frac{1}{3}\left[\left(\frac{\Delta x}{2}\right)^2 \bar{u}_x\, \bar{v}_x + \left(\frac{\Delta y}{2}\right)^2 \bar{u}_y\, \bar{v}_y\right] \tag{2.31}$$

$$\tau^{yy} = -\frac{1}{3}\left[\left(\frac{\Delta x}{2}\right)^2 \bar{v}_x^2 + \left(\frac{\Delta y}{2}\right)^2 \bar{v}_y^2\right]. \tag{2.32}$$

Here the (Cartesian) tensor indices are shown as superscripts to distinguish them from the subscripts that denote spatial differentiation.

Fourth, we emphasize the similarity of this SGS tensor to the LES model of Clark – see, for example, page 628 in Pope (2000). This model belongs to the class of similarity models, which are found to accurately represent the nonlinear dynamics and energy transfer of turbulence in simulations, but which are generally not sufficiently dissipative. The Clark model is often used in conjunction with Smagorinsky to form mixed models (cf. Pope 2000 or Meneveau and Katz 2000).

Finally, we call attention to the fact that the finite-scale equations depend sensitively on the length scales of the averaging. We emphasize that these are not intrinsic scales of the flow, but in fact *represent the length scales of the observer*. From a physics point of view, an observer measures aspects of a flow using experimental apparatus that itself has finite scales – such as the diameter of a wire, the response time of a detector, and so on. The fact that the equations and their solutions change as the length scales change is not a flaw, but a necessary consequence of their interpretation as a model of reality, as measured by a particular observer.

2.4 NFV modified equation

In this section, we will compare the finite-scale equation derived in the previous section with the MEA of a particular NFV scheme, MPDATA (Chapter 4d). MPDATA has been used successfully in ILES simulations of the atmosphere, both on mesoscale and global-scale problems; some examples are described in Chapter 14.

MPDATA is constructed directly by using the properties of iterated upwinding, in contrast to the majority of NFV schemes, which are based on the idea of flux limiting. Nevertheless, MPDATA's properties, as exposed by MEA, are typical of many NFV schemes. In the next section, we will delineate the common features that make for successful ILES as well as important distinctions that relate to the dissipative process.

2.4.1 Implicit SGS stresses

Modified equation analysis is a technique for generating a PDE whose solution closely approximates the solution of a numerical algorithm. Comparison of the MEA of an algorithm with its model PDE gives useful information about the accuracy and the stability of the algorithm. A description of this important technique can be found in Chapter 5 of this volume and associated references.

We will assume a simple data structure where both components of velocity are located at the cell centers. A straightforward, if somewhat tedious, Taylor analysis of the MPDATA algorithm applied to the 2D Navier–Stokes equations, (2.5), leads to the modified equations. Here, we focus only on the semidiscrete equations by letting the time step $\Delta t \to 0$, to correspond to the finite-volume equations (2.21) and (2.22) where we did only spatial averaging. Also, we exhibit only the truncation terms originating in the advective terms, to allow direct comparison with the finite-scale "subgrid stress" terms in (2.30) through (2.32). It turns out that these truncation terms also can be written as the divergence of a tensor. To lowest order, the implicit subgrid stress $\mathcal{T}$ of the MPDATA algorithm is

$$\mathcal{T}_{xx} = \left[\frac{1}{4}u_x\,|u_x| + \frac{1}{12}u_x\,u_x + \frac{1}{3}u\,u_{xx}\right]_x \Delta x^2 \tag{2.33}$$

$$\mathcal{T}_{xy} = \left[\frac{1}{4}u_y\,|v_y| + \frac{1}{12}u_y\,v_y + \frac{1}{6}(u\,v_{yy} + v\,u_{yy})\right]_y \Delta y^2 \tag{2.34}$$

$$\mathcal{T}_{yx} = \left[\frac{1}{4}v_x\,|u_x| + \frac{1}{12}u_x\,v_x + \frac{1}{6}(u\,v_{xx} + v\,u_{xx})\right]_x \Delta x^2 \tag{2.35}$$

and

$$\mathcal{T}_{yy} = \left[\frac{1}{4}v_y\,|v_y| + \frac{1}{12}v_y\,v_y + \frac{1}{3}v\,v_{yy}\right]_y \Delta y^2. \tag{2.36}$$

Let us now do a detailed comparison between the finite-scale SGS stress of equations (2.30) through (2.32) and the implicit SGS stress of equations (2.33) through (2.36).

First of all, we note that the truncation terms can be written as a second-order tensor. This is a direct consequence of the finite-volume nature of the approximation and underlines the importance of the "FV" in NFV methods.

Second, we note that each of the components in $\mathcal{T}$ is quadratic in Δx or Δy, similar to the properties of τ. This is a direct consequence of the second-order accuracy of MPDATA and explains why first-order schemes such as donor cell are not suitable for ILES, even though they are nonoscillatory. Perhaps of equal importance is the implication that higher-order (than second) schemes will not have the proper dimensional dependence and are also unsuitable for ILES.

Third, we note that $\mathcal{T}$ is not symmetric in its off-diagonal components, whereas τ is symmetric. More generally, we may note the lack of certain terms in $\mathcal{T}$ that are present in τ. For example, there are no terms of order Δy^2 in $\mathcal{T}_{xx}$. This source of this deficit is easy to uncover, and in fact results from the particular form used by MPDATA to estimate the velocity at the center of the edge of a computation cell, specifically the average of the two values of the adjacent cells. This ignores the perpendicular variation of these values. This is also a relatively easy deficiency to fix. In computational experiments, however, we have seen little difference when "fuller" stencils are used for this averaging, indicating a relative lack of importance of these terms.

2.4.2 Energy analysis and computational stability

Both the finite-scale subgrid stresses, (2.30) through (2.32), and the implicit subgrid stresses, (2.33) through (2.36), are just the lowest order in an infinite series of terms with higher-order derivatives and larger (even) powers of Δx and Δy. Our assumptions about the smoothness of the averaged flow are designed to imply that these higher-order terms can be ignored *from the point of view of accuracy*. Stability of the equations is an independent issue. Stability can be studied through the energy equation.

The total rate of inviscid energy dissipation – that is, independent of the physical viscosity ν – is

$$\frac{dE}{dt} = \frac{1}{2} \int_D \left[u\, \tau_x^{xx} + u\, \tau_y^{xy} + v\, \tau_x^{xy} + v\, \tau_y^{yy}\right] dx\, dy, \tag{2.37}$$

where D is the two-dimensional domain. Integrating by parts and neglecting surface terms (work done by external forces) yields

$$\frac{dE}{dt} = -\frac{1}{2} \int_D [u_x\, \tau^{xx} + u_y\, \tau^{xy} + v_x\, \tau^{yx} + v_y\, \tau^{yy}]\, dx\, dy. \tag{2.38}$$

Substituting the finite-scale subgrid stresses into (2.38) yields:

$$\frac{dE_{\rm FS}}{dt} = \frac{1}{6}\left(\frac{\Delta x}{2}\right)^2 \langle \bar{u}_x^3 \rangle + \frac{1}{6}\left(\frac{\Delta y}{2}\right)^2 \langle \bar{v}_y^3 \rangle + \frac{1}{6}\left[\left(\frac{\Delta x}{2}\right)^2 - \left(\frac{\Delta y}{2}\right)^2\right] \langle \bar{u}_x \bar{u}_y \bar{v}_x \rangle. \tag{2.39}$$

Here the brackets indicate spatial integration over the domain. Note that for solutions (u, v) of NSE, $\langle u_x^3 \rangle < 0$ and $\langle v_y^3 \rangle < 0$ by Kolmogorov's 4/5 law; these inequalities are verified computationally in Chapter 14 for MPDATA solutions of decaying turbulence. In an isotropic flow $\langle \bar{u}_x \bar{u}_y \bar{v}_x \rangle$ would vanish. Thus, in the absence of forces, kinetic energy is absolutely decreasing and the (truncated) finite-volume equations are globally stable.

Next, substituting the implicit subgrid stresses of the modified equations into (2.38) yields

$$\begin{aligned}
\frac{dE_{\mathrm{ME}}}{dt} &= \left(\frac{\Delta x^2}{2}\right)\left[\frac{1}{3}\left\langle \bar{u}_x^3 \right\rangle - \left\langle |\bar{u}_x^3| \right\rangle + \frac{1}{3}\left\langle \bar{u}_x \bar{v}_x^2 \right\rangle - \left\langle |\bar{u}_x| \bar{v}_x^2 \right\rangle\right] \\
&+ \left(\frac{\Delta y^2}{2}\right)\left[\frac{1}{3}\left\langle \bar{v}_y^3 \right\rangle - \left\langle |\bar{v}_y^3| \right\rangle + \frac{1}{3}\left\langle \bar{v}_y \bar{u}_y^2 \right\rangle - \left\langle |\bar{v}_y| \bar{u}_y^2 \right\rangle\right] \\
&- \left(\frac{\Delta x^2}{3}\right)\left[\langle \bar{v}\bar{v}_x \bar{u}_{xx} \rangle - \langle \bar{u}\bar{v}_x \bar{v}_{xx} \rangle\right] \\
&- \left(\frac{\Delta y^2}{3}\right)\left[\langle \bar{u}\bar{u}_y \bar{v}_{yy} \rangle - \langle \bar{v}\bar{u}_y \bar{u}_{yy} \rangle\right]. \qquad (2.40)
\end{aligned}$$

We note the similarities to (2.39), and proceed to discuss the differences next.

The NFV methods are nonlinearly stable by construction. This can be seen in (2.40), where several of the terms can be grouped to ensure that the integrands are negative definite – for example, $\langle \frac{1}{3}\bar{u}_x^3 - |\bar{u}_x^3| \rangle < 0$. This is a different kind of stability from that of the finite-scale equations, as it does not depend on the solution. In the language of numerical analysis, the MPDATA modified equations for the NSE are locally stable, whereas the finite-scale equations are globally stable.

Based on the energy analysis, the MPDATA implicit subgrid stress tensor can be written as the sum of two parts, one of which is absolutely dissipative and one of which corresponds to the corrective terms of the finite-scale equation. In the case of MPDATA, the dissipative stress is similar to a tensor version of the common Smagorinsky model. As we remarked in Section 2.4, the nonlinear terms are the same as those of the self-similar Clark model (Pope 2000). Thus, *MPDATA has the form of a mixed LES model.*

2.5 A Discussion of energy dissipation

Successful ILES simulations have been found to be a property of most, but not all, NFV algorithms. This does not imply that the results of using different NFV algorithms are entirely equivalent. In this section, we discuss the differences among these results. The conceptual framework of this discussion requires us to delve more deeply into the details of the numerical regularization. A computational validation of our discussion and conclusions in this section is presented in Chapter 5.

The theoretical analysis of Section 2.3 and the comparisons with the MPDATA-modified equation in Section 2.4 suggest that it is possible to identify the essential algorithmic elements required for ILES. We begin by summarizing these elements:

- The first element is the appearance of the self-similar term (i.e., Clark model) in the MEA of the algorithm. It is not difficult to show that the presence of this term is a direct consequence of finite-volume differencing. This term scales generically like the square of a characteristic length scale, h, of the averaging volume, such as Δx^2 or Δy^2 in two-dimensional simulations.
- The second element is the presence of sufficient dissipation to "regularize" the equations. A corollary to this is that there should not be too much dissipation – that is, should not dominate the self-similar term. In our analysis of MPDATA, we found the dissipation also scales like h^2; in fact, is comparable in size in regions of compression, but vanishes in regions of expansion.

Although most NFV schemes can be used for ILES, there are differences among the results. In particular, one might suppose that there are advantages to NFV algorithms whose dissipation scales with a higher power of h, which may minimize the interaction with the self-similar term. It is possible to test this hypothesis within the context of MPDATA, which has an option to specify the number of corrective iterations used. This option, termed IORD, is described in Chapter 4d and involves iterating the basic scheme to further reduce the simulation error. When IORD = 1, the algorithm is a simple donor cell, which is found to be too diffusive for ILES. When IORD = 2, the scheme described in Section 2.5 results. When IORD = 3, dissipation is further reduced; for comparison with equation (2.33), the particular subgrid stress component $\mathcal{T}_{xx}$ has the modified form

$$\mathcal{T}_{xx} = \left(\frac{1}{12} u_x\, u_x + \frac{1}{3} u\, u_{xx}\right)_x \Delta x^2 + \mathcal{O}(\Delta x^3) + \frac{1}{6}\,\mathrm{sgn}\,(u_x)\, u_{xx}^2\, \Delta x^4, \tag{2.41}$$

where $\mathrm{sgn}\,(u_x) \equiv \frac{|u_x|}{u_x}$. The terms $\mathcal{O}(\Delta x^3)$ are not dissipative; the first locally dissipative term shows up at fourth order (other fourth-order terms also are present but are not dissipative). In general, incrementing IORD by 1 preserves the self-similar term while increasing the order of dissipation by 2.

The effect of increasing the order of dissipation in MPDATA simulations is studied in Chapter 5. To summarize these results, the difference between IORD = 2 and IORD = 3 is substantial, both in the mean flow characteristics and in the intermittency. The further increase to IORD = 4 and above has minimal effect on the results. This latter result is a little surprising, and is important to understand as a limitation of the MEA approach. In the simulation, energy is dissipated in regions of steep compressive gradients and also at local extrema. Taylor expansion, which underlies MEA, is not sufficiently convergent to allow an accurate representation of the equations at sharp extrema.

To demonstrate the importance of dissipation at extrema, we have also included simulations in Chapter 5 using a monotonicity-preserving scheme with fourth-order dissipation equivalent to MPDATA with IORD = 3. To summarize these comparisons, the results of the monotonicity-preserving scheme results show a better agreement with mean flow characteristics than MPDATA, but show substantially less intermittency. The latter results give some insight into a question that will also surface elsewhere in this volume (Chapter 8) – namely, is the strict preservation of monotonicity an ingredient for optimal ILES, or are weaker conditions such as sign preservation or positivity preferable? In particular, it is clear that different NFV schemes provide qualitatively different implicit models by which SGS fluctuations affect the resolved flow features. The apparent conclusion is that each approach has potential advantages for particular problems, and so there is no optimal scheme for all problems; the choice of NFV scheme should depend on the specific questions that a simulation is meant to address.

2.6 Summary

Our goal in this chapter has been to provide a rationale for the ILES approach. Our strategy has been to argue that the finite-volume Navier–Stokes equations are the most appropriate model for simulating turbulent flows, to derive these for the case of the 2D Navier–Stokes equation, and to show that a particular numerical algorithm, MPDATA, is effectively solving these equations. We also exposed the connection of the implicit subgrid model of MPDATA to the class of mixed models in explicit LES. We will extend these ideas more generally to other methods of the class of NFV schemes in the next three chapters. In Chapter 3, we will provide more detailed background on the explicit LES approach, the ideas that underpin it, and some of the methodologies it includes. In Chapter 4, we will provide more detailed descriptions of the particular NFV schemes that are used in the body of the volume. Although all belong to the general class of NFV methods, we will see that the underlying concepts are quite varied. Then, in Chapter 5, we will draw out the common threads of these schemes and elucidate the features necessary for successful ILES. In closing and further integrating this section on *Capturing Physics*, Chapter 6, by Adams, Hickel, and Domaradzki, describes how the approximate deconvolution method can be used as a powerful bridge connecting LES and ILES.

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