

EFFECTIVE SUBGRID MODELING FROM THE ILES SIMULATION OF COMPRESSIBLE TURBULENCE

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Abstract. *Implicit large eddy simulation (ILES) has provided many computer simulations with an efficient and effective model for turbulence. The capacity for ILES has been shown to arise from a broad class of numerical methods with specific properties producing non-oscillatory solutions using limiters that provide these methods with nonlinear stability. The use of modified equation has allowed us to understand the mechanisms behind the efficacy of ILES as a model. Much of the understanding of the ILES modeling has proceeded in the realm of incompressible flows. Here, we extend this analysis to compressible flows. While the general conclusions are consistent with our previous findings the compressible case has several important distinctions. Like the incompressible analysis, the ILES of compressible flow is dominated by an effective self-similarity model [1, 3, 24].*

Here, we focus on one of these issues, the form of the effective subgrid model for the conservation of mass equations. In the mass equation, the leading order model is a self-similarity model acting on the joint gradients of density and velocity. The dissipative ILES model results from the limiter and upwind differencing resulting in effects proportional to the acoustic modes in the flow as well as the convective effects. We examine the model in several limits including the incompressible limit. This equation differs from the standard form found in the classical Navier-Stokes equations, but generally follows the form suggested by Brenner [5] in a modification of Navier-Stokes necessary to successfully reproduce some experimentally measured phenomena. The implications of these developments are discussed in relation to the usual turbulence modeling approaches.

1 Introduction

ILES has provided both a powerful and practical approach to modeling turbulence in a broad variety of circumstances. Successful ILES modeling has been conducted with a variety of high-resolution methods. The first observation of effective modeling of turbulence without explicit modeling is credited to Jay Boris [4] who called the methodology MILES for Monotonically integrated large eddy simulation. Boris applied the flux-corrected transport method that he had developed to produce MILES. Other researchers also found the same capacity with other methods. Paul Woodward applied the Godunov-type method PPM (piecewise parabolic method) to astrophysical problems and discovered effective turbulence modeling [26]. David Youngs found similar results with an entirely different class of methods using a Lagrange-Remap methodology [20]. More recently, success has been had with TVD methods for engineering flows [15]. These methods have now been documented in several review articles [9, 10] and two books [11, 16]. These two articles and books catalog the large variety of methods and applications where ILES has had success.

Going back to the origins of numerical fluid dynamics provides more compelling evidence that ILES and classical LES are connected. The original shock capturing method developed by Von Neumann and Richtmyer [31] used a nonlinear artificial viscosity to stabilize the computation of shock waves. This same nonlinear viscosity was then applied in weather modeling by Joseph Smagorinsky albeit in three dimensions [29, 30]. Smagorinsky's viscosity was the original subgrid modeling used for LES. Thus, classical LES has its origins with the first nonlinear shock capturing method that has ultimately developed into the same class of methods now associated with ILES.

We have examined a number of high-resolution methods using the technique known as modified equation analysis (MEA) [21, 22, 23, 27]. MEA produces the differential equation more accurately solved by a numerical method than the original intended equation. For example, first-order upwind differencing of the simple advection equation produces the solution to a specific advection-diffusion equation. Through MEA we have uncovered the form of the implicit model from which ILES's modeling success is derived. In the following sections we will describe the MEA analysis of compressible flow and discuss the implications for the form of the implicit model. The differences with classical modeling is most acute in the mass equation. This allows us to focus on how ILES provides a unique and powerful modeling technique.

2 Modified Equation Analysis

MEA was first developed to assess the stability of numerical algorithms [18]. Basically, the analysis consists of Taylor series expansion about a relevant mesh spacing $\Delta x \rightarrow 0$ applied to the discrete terms of the algorithm as if the equation (and its solution) were continuous. We note that the limit of $\Delta x \rightarrow 0$ cannot be achieved in reality (not to mention the violation of the continuum hypothesis that the equations themselves are

based upon). This immediately raises the issue of the dynamics at finite scales, which we examined in the paper [23]. We found that the physics of finite volumes of fluid evolve by different evolution equations than the Navier-Stokes equations. This is predicated on the presence of dissipation that enforces the smoothness of the flow at small scales. A renormalization procedure allows the smoothness to insure the applicability of the Taylor series expansion at each succeeding scale. We note that numerical viscosity insures that a comparable result will apply to ILES solutions. The techniques that produce the nonlinear stability of the methods also work to insure that the solutions are smooth enough for the Taylor series expansion to have an explanatory power undiluted by the presence of discontinuities and unresolved layer in a flowfield.

The main assumption is the use of Taylor analysis itself, which implies restrictions on the smoothness of the function. In particular, the Taylor analysis produces an infinite series of terms, but the modified equation is formed by truncating this series and keeping only the lowest order terms which are assumed to dominate the numerical effects. Our analysis indicates that numerical dissipation is sufficient to keep the flowfield regular enough for the Taylor series expansion to have meaning. A discussion of the uses of MEA and caveats of its use can be found in [21].

The modified equation for a *consistent* algorithm consists of the modeled PDE plus additional terms, each proportional to a power of the computational time step Δt or of the computational cell size Δx , or possibly both. The smallest power among these terms determines the order of accuracy of the scheme. In general, if the PDE has the form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = 0, \quad (1)$$

then the modified equation of a consistent algorithm will have the form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \mathbf{T}(\mathbf{U}, \Delta x, \Delta t), \quad (2)$$

where \mathbf{T} is the truncation term. More specifically, when finite volume differencing¹ is employed, then the modified equation will have the form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \nabla \cdot \boldsymbol{\tau}(\mathbf{U}, \Delta x, \Delta t). \quad (3)$$

This produces the result in a form similar to that found in standard constitutive modeling with a stress tensor. *Thus, all algorithms based on finite-volume differencing have a truncation term in the form of the divergence of a "subgrid scale" model.* The conditions under which this form is useful for ILES is the main subject of this paper. We will focus on the compressible form of the stress tensor associated with the mass (or continuity) equation.

¹Finite volume differencing is also known as conservative form and as flux form differencing. We will use these terms interchangeably.

3 Multidimensional MEA Analysis

It is straightforward to extend the one-dimensional analysis to fully three-dimensional algorithms. In this section, we will show the general results assuming the use of a second-order, but otherwise unspecified flux limiters for both incompressible and compressible flows in 3-D. First, the 3-D incompressible Euler equations will be presented using a general limiter that provides a nonlinear combination of a first-order and second-order methods. We follow this with a presentation of the modified equation for the fully compressible version of the same method.

We will derive the modified equation using symbolic algebra software, specifically the Mathematica program. We will use tensor notation with implied summation over repeated indices. For the case of incompressible flow, we will then specialize our results to the two-dimensional case on a rectangular mesh of cells Δx by Δy by Δz . This will allow detailed comparisons of our results with those in [23] for the finite scale equations and for the modified equation of the MPDATA algorithm.

The incompressible Euler equations can be written compactly as

$$\frac{\partial u_m}{\partial t} + \frac{\partial u_n u_m}{\partial x_n} + \frac{\partial p}{\partial x_m} = 0, \quad (4)$$

where the indices $m, n = 1, 2, 3$ indicate summation over those indices. The constraint of incompressibility is expressed by

$$\frac{\partial u_n}{\partial x_n} = 0. \quad (5)$$

The compressible equations can also be written abstractly. Our notation will employ the vector flux function of a vector of conserved quantities,

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x_n} = 0. \quad (6)$$

This represents a system of conservation laws.

In the analysis that follows the pressure field is defined as a potential field that acts to ensure that the velocity field is divergence-free (i.e., solenoidal). Our algorithm will consist of the combination of a first-order and a second-order accurate method, with relative weights of the two schemes determined by a flux-limiter function. We construct a second-order accurate method by defining a set of edge variables as the averages of the cell-centered values across a cell-edge, i.e.,

$$\begin{aligned} u_{m,i+\frac{1}{2},j,k} &= \frac{1}{2} (u_{m,i,j,k} + u_{m,i+1,j,k}), \\ u_{m,i,j+\frac{1}{2},k} &= \frac{1}{2} (u_{m,i,j,k} + u_{m,i,j+1,k}), \\ u_{m,i,j,k+\frac{1}{2}} &= \frac{1}{2} (u_{m,i,j,k} + u_{m,i,j,k+1}), \end{aligned} \quad (7)$$

Here i, j, k are the grid indices associated with the cell centers. The numerical approximation for the divergence is

$$\begin{aligned} & \frac{u_{1,i+\frac{1}{2},j,k} - u_{1,i-\frac{1}{2},j,k}}{\Delta x_1} + \frac{u_{2,i,j+\frac{1}{2},k} - u_{2,i,j-\frac{1}{2},k}}{\Delta x_2} + \\ & \frac{u_{3,i,j,k+\frac{1}{2}} - u_{3,i,j,k-\frac{1}{2}}}{\Delta x_3} = 0. \end{aligned} \quad (8)$$

The second-order expression for the nonlinear product that appears in the advective terms is simply constructed as the product of the edge values, e.g.,

$$(u_1 u_2)_{i+\frac{1}{2},j,k}^{2\text{nd}} = u_{1,i+\frac{1}{2},j,k} u_{2,i+\frac{1}{2},j,k}. \quad (9)$$

With our second-order approximations defined, we need to define the first-order approximations. This is done using the donor cell method where the numerical definition of the edge value is biased by the normal velocity. For example in direction 1 for the 2 motion equation we need to define the product $u_1 u_2$ at cell boundaries,

$$(u_1 u_2)_{i+\frac{1}{2},j,k}^{1\text{st}} = (u_1 u_2)_{i+\frac{1}{2},j,k}^{2\text{nd}} - \frac{1}{2} |u_{1,i+\frac{1}{2},j,k}| (u_{2,i+1,j,k} - u_{2,i,j,k}). \quad (10)$$

We will define our limiter abstractly as a function, ϕh that depends on the mesh spacing $h = \Delta x_m$ (we assume that the mesh spacing is constant, but not necessarily equal, in all three directions for simplicity). Although the flux limiter is itself dimensionless, we have explicitly factored out the cell dimension in anticipation of future results. A number of limiters could fit this general form including the MPDATA method, Sweby's form of TVD methods, high-order Godunov methods and flux-corrected transport to mention but a few.

With the limiter defined we can simply express our high resolution method using a combination of the two previous expressions,

$$(u_1 u_2)_{i+\frac{1}{2},j,k}^{\text{ hires }} = \phi_1 h_1 (u_1 u_2)_{i+\frac{1}{2},j,k}^{1\text{st}} + (1 - \phi_1 h_1) (u_1 u_2)_{i+\frac{1}{2},j,k}^{2\text{nd}}. \quad (11)$$

With our basic numerical method defined, we introduce our numerical approximations into the discrete incompressible Euler equations and expand using a Taylor series in each of the three coordinate directions. After some simplification our results are compactly written notation as

$$\begin{aligned} & \frac{\partial u_m}{\partial t} + \frac{\partial u_n u_m}{\partial x_n} + \frac{\partial p}{\partial x_m} \\ & = h_n^2 \left[\frac{1}{2} \phi_n |u_n| \left(\frac{1}{u_n} \frac{\partial u_n}{\partial x_n} \frac{\partial u_m}{\partial x_n} + \frac{\partial^2 u_m}{\partial x_n^2} \right) + \frac{1}{2} |u_n| \frac{\partial \phi_n}{\partial x} \frac{\partial u_m}{\partial x_n} \right. \\ & \quad \left. - \frac{1}{4} \left(\frac{\partial u_m}{\partial x_n} \frac{\partial^2 u_n}{\partial x_n^2} + \frac{\partial u_n}{\partial x_n} \frac{\partial^2 u_m}{\partial x_n^2} \right) - \frac{1}{6} \left(u_n \frac{\partial^3 u_m}{\partial x_n^3} + u_m \frac{\partial^3 u_n}{\partial x_n^3} \right) \right] \\ & \quad + \mathcal{O}(h_n^3), \end{aligned} \quad (12)$$

where again the pressure gradient is simply the gradient of the potential function that enforces the discrete divergence condition, (9). This form is similar to the one-dimensional forms in the presence of the self-similar terms and in the leading order impact of the limiter on the dissipation.

The entire approach has been successfully validated using detailed data from high Reynolds number decaying turbulence [19]. The validation has included integral behavior such as kinetic energy decay, and energy spectra as well as velocity PDFs [23, 27]. In all cases the ILES methods produced exceptional results despite the relatively coarse grids. Furthermore the ILES methods produced a far better reproduction of the intermittency measured in the experiment than the classical LES methods tested by [19]. In an overall sense, the ILES models appear to have achieved a favorable validation against experimental data.

4 Analysis of Compressible ILES

We can apply the same basic differencing for compressible flows. The key differences are the lack of the divergence-free constraint and the application of the differencing to a vector function with an abstractly defined flux function. The high-order flux (second-order) is defined using the face-averaged value as before, but now is written

$$\mathbf{f}_{i+half,j,k}^{2nd} = \mathbf{f} \left(\mathbf{u}_{i+\frac{1}{2},j,k} \right) \quad (13)$$

The first order flux is defined with the help of the flux Jacobian, $\mathbf{f}' = \partial \mathbf{f} / \partial \mathbf{u}$ as,

$$\mathbf{f}_{i+half,j,k}^{1st} = \mathbf{f}_{i+half,j,k}^{2nd} - \frac{1}{2} |\mathbf{f}'| (\mathbf{u}_{i+1,j,k} - \mathbf{u}_{i,j,k}). \quad (14)$$

Substituting these expressions combined using our abstractly defined limiter that blends the first and second-order fluxes and expanding the expression in a three-dimensional Taylor series produces,

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x_n} & \quad (15) \\ &= h_n^2 \frac{\partial}{\partial x_n} \left[\frac{1}{2} \phi_n |\mathbf{f}'| \frac{\partial \mathbf{u}}{\partial x_n} - \frac{1}{6} \mathbf{f}' \frac{\partial^2 \mathbf{u}}{\partial x_n^2} - \frac{1}{24} \mathbf{f}'' \left(\frac{\partial \mathbf{u}}{\partial x_n} \right)^2 \right] \\ &+ \mathcal{O}(h_n^3). \end{aligned}$$

This form is also similar to the one-dimensional compressible analysis having the self-similar terms proportional to the convexity of the flux function (\mathbf{f}''). The limiter enters in to the analysis as expected at second-order.

By substituting our defined high-resolution method specifically for the mass (continuity) equation we produce the following form,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} = h_n^2 \frac{\partial}{\partial x_n} \left[\frac{\phi_n |u_n|}{2} \frac{\partial (\rho - p/a^2)}{\partial x_n} \right] \quad (16)$$

$$\begin{aligned}
 & + \frac{\phi_n |u_n - a|}{4} \frac{\partial (\rho u_n / a - p / a^2)}{\partial x_n} + \frac{\phi_n |u_n + a|}{4} \frac{\partial (\rho u_n / a + p / a^2)}{\partial x_n} \\
 & - \frac{u_n}{6} \frac{\partial^2 \rho}{\partial x_n^2} - \frac{\rho}{6} \frac{\partial^2 u_n}{\partial x_n^2} \\
 & - \left. \frac{\gamma + 1}{48} \frac{\partial \rho}{\partial x_n} \frac{\partial u_n}{\partial x_n} \right] + \mathcal{O}(h_n^3).
 \end{aligned}$$

Here a is the sound speed.

Note that the form has the self-similarity term and a nonlinear dissipation from the upwind differencing, which upon further analysis comes directly from the acoustic waves. For the mass equation, the effective subgrid model is quite unlike that found in classical LES modeling. Specifying the above analysis for the mass equation and providing an upwinding mechanism that operates characteristic-by-characteristic (for a gamma law gas) gives, If we take the limit where the sound speed becomes very large in comparison to the fluid velocity, the dissipation remains,

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} & \tag{17} \\
 = h_n^2 \frac{\partial}{\partial x_n} \left[\frac{1}{2} \phi_n \rho \frac{\partial u_n}{\partial x_n} - \frac{\rho}{6} \frac{\partial^2 u_n}{\partial x_n^2} - \frac{\gamma + 1}{48} \frac{\partial \rho}{\partial x_n} \frac{\partial u_n}{\partial x_n} \right] + \mathcal{O}(h_n^3).
 \end{aligned}$$

Thinking about the mixing of fluids of different densities, the right hand side makes physical sense. The stretching for fluid elements by the velocity field will act to mix the fluid at the large scale bringing fluids of differing density into contact on the scale of fluid volumes parameterized by h .

The bottom line is that the mass equation has both a nonlinear dissipative model and a self-similar model under all relevant circumstances. As a specific example the shock capturing LES model by Cook and Cabot [8] has a zero right hand side for the mass equation (Florina and Lele have modified this method to include a non-zero right hand side [12]). Cook and Cabot are following a tried principle of connecting the turbulent closure's form to that of the Navier-Stokes. As such the physical interpretation remains firmly connected to our understanding of the basic PDEs and laminar flow.

We will relay recent developments regarding the form of the mass equation in the Navier-Stokes equation. These developments have been spearheaded by Howard Brenner of MIT and have reformulated the Navier-Stokes equations in terms of a volumetric velocity rather than a mass velocity. The bottom line of this reformulation is to introduce a diffusive component into the mass equation. Secondly, we might be tempted to ask whether the effective governing equations for turbulent flows in finite volumes of fluid ought to have the same form as the equations governing the laminar flow at a point? Our suggestion is that they should not, for several important and valid reasons.

5 Discussion of the MEA Analysis of the Mass Equation

Unlike most classical turbulence models, the continuity equation has a non-zero right hand side. We note that techniques such as Favre averaging usually produce a form for the continuity equation that is identical to the standard continuity equation with zero right hand side. It is notable that many of the early applications of ILES have been to material mixing where there are clearly nonlinear effects from density and velocity fluctuations. These effects are notably lacking from standard turbulence modeling approaches although many models will include these effects in the momentum and energy balances. Until recently the modeling approach ILES could be criticized for having a form so different than the Navier-Stokes equation. A common approach is to have the constitutive modeling follow the same form as physical properties. Evidence now exists that calls this critique into question.

It is notable that the form of the continuity equation has been the subject of vigorous debate recently. The challenges to the classical form have been summarized in a remarkable sequence of papers by Brenner [5, 2, 6, 7]. In these papers compelling evidence is presented that the Navier-Stokes equations for compressible flows are missing a key physical mechanism for mass transfer. This is a diffusive mechanism that is necessary to provide a systematic explanation of experimental data. In simple terms, the convective fluxes of mass exchange atoms or molecules with the surrounding fluid, thus variations in the rate of exchange would naturally lead to diffusive fluxes. This explanation is equivalent to the classical explanation of diffusion rates in gases and liquids. A nonzero diffusion rate would only be physical under the conditions that the material were solid and the flux volumes were impermeable.

We make a particular point of concentrating on this result in that our analysis systematically produces a continuity equation with a non-zero right hand side. This is true for all methods that have been useful as ILES techniques and has its basis in the form for the equations controlling the evolution of volumes of fluid [23]. Bringing the recent developments to mind shows that the ILES approach follows directly from parallel physical arguments. One stems from the small scale physics leading to diffusion through random motion of the constituent particles comprising the flow. The second stems from the nature of the evolution of finite volumes of fluid. These finite volumes are a natural state to examine fluid flows due to the existence of finite scales of observation associated with experimental techniques. The closure to these ideas follows the association of finite scales of observation with the use of finite volume (or conservative) methods. Finite volume methods also need to employ some sort of instantiation of the second law of thermodynamics to provide the guarantee of physical solutions. The second law of thermodynamics follows from a dissipative or diffusive impact on the large scale solution to equations (via a vanishing viscosity solution).

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