Numerical Simulation of Supersonic Flows

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Abstract

The goal of this study is to present a perspective of the current status of Large Eddy Simulation (LES) of gas flows. Emphasis is given to the minimum requirements a numerical simulation method should have, both from the algorithm and from the modeling standpoint. The problems that need to be solved in order to perform LES of supersonic flows are also addressed.

1 Introduction

Even after a couple of decades of steady progress of both algorithms and available computer power, the Direct Numerical Simulation (DNS) of the governing equations for a gas flow – the Navier-Stokes equations – remains too costly to be applied to problems of practical interest. Indeed, most engineering systems currently in use involve turbulent flows, where the Reynolds number is very large (of the order of 10^7 or more). As a consequence, several orders of magnitude separate the largest length scales present in the flowfield from the smallest ones: the ratio between the so-called integral length scale and the Kolmogorov (or dissipation) micro-scale is proportional to $\mathrm{Re}^{9/4}$. Therefore, DNS is limited, in the near future, to flow configurations of academic interest only. Nevertheless, DNS has proven to be an interesting tool for the development and *a priori* testing of turbulence models.

A classical approach used to overcome such a limitation is the Reynolds (or time) averaging of the Navier-Stokes (RANS) equations. This technique decomposes each flow variable (velocity, density, etc.) in average and time-fluctuating parts. The equations are then averaged, resulting in a number of unknown (or unclosed) terms which involve averages of products of fluctuating quantities. These terms are usually represented by models which are based on phenomenological assumptions, and thus very often must be adapted depending on the class of flowfield (*i.e.* on the geometry) involved. Another drawback of this approach is its inherent inability to deal with flows that contain some kind of periodic motion which carries a large amount of energy, e.g. vortex sheets.

A technique which may be able to circumvent some of the shortcomings of the RANS simulations, at a reasonable computational cost, is the Large Eddy Simulation. LES involves space filtering of the Navier-Stokes equations which also leads to unclosed terms, but yield an accurate representation of the flowfield time scales. Such unclosed terms are commonly referred to as Subgrid Scale (SGS) stresses, since they represent correlations between the unresolved flowfield spatial scales. The underlying assumption here is that turbulent phenomena at the very small scales possess a behavior which is independent of the largest (resolved) scales of the flowfield. In particular, it is generally assumed that the energy spectrum of the smallest eddies varies as $k^{-5/3}$, where k is the wavenumber of the eddies. Thus, the closure of the SGS terms attempt to mimic these small-scale invariant motions, and also the energy transfer across resolved and unresolved scales. Even if LES has received considerable attention in the past few years, stemming from metereological to engineering type flows, it is far from being a mature approach.

In what follows, it is first presented a short review of the recent literature on LES. The different requirements that both the SGS models and the solution algorithm should satisfy are highlighted. Then the filtered equations for compressible flows are given, and the different unclosed terms are shown. Finally, guidelines for future works on this field are suggested.

2 Literature Review

Since the extensive review of early work on LES by Rogallo and Moin (1984), several papers summarize the advances in this field. Lesieur and Métais (1996) and Lesieur (1997) present the formalism involved in filtering the Navier-Stokes equations. The various models proposed to close the subgrid scale stresses are also discussed: Smagorinsky models, spectral eddy viscosity models, structure function models, scale similarity models and dynamic models. In each case, both the advantages and the drawbacks of each model are presented, together with illustrative examples. Some attention is also given to numerical diffusion issues. Speziale (1998) proposes a closure of the model equations that could diminish the gap existing between RANS computations and LES. After presenting the filtered equations and the different SGS closures developed, Piomelli (1999) discusses the successes in predicting different types of flow configurations and the various steps to come before LES can be used as a reliable engineering predictive tool. In particular, he emphasizes the need for a better prediction of turbulence decay near walls, the challenges involved in closing SGS terms in compressible flows and also the problems encountered in acoustic modeling. Meneveau and Katz (2000) present a review of *a priori* and *a posteriori* studies of the different SGS models. They also stress the need for more comparisons between LES and experimental data in order to validate and subsequently improve SGS closures. Accordingly, recently built facilities, as the one of Besson *et al.* (2000), have been designed and are being used with the specific objective of comparisons with LES. The review papers above cited clearly show that, even if substantial progress has been achieved in developing and testing SGS closures, there is a lack of systematic and thorough comparisons between the different models in various flow configurations.

Concerning the numerical modeling aspects of LES, the work of Ghosal and Moin (1995) discusses the use of filters of variable width and the errors introduced by commuting filtering and differentiation operations. In particular, they develop corrections to the equations that account for the commuting error with a given accuracy. Subsequently, Ghosal (1996) performed a comparative study of the errors introduced by the filtering and the discretization. It was shown that the numerical discretization errors remain larger than the SGS force even for eight-order accuracy numerical methods. A strategy to overcome this problem was introduced based on filters widths larger than the grid size. As it was also stressed by Garnier *et al.* (1999), an essential requirement that a numerical scheme must satisfy in order to be used for LES is that either the numerical dissipation is smaller than the SGS or the numerical dissipation correctly reproduces the SGS behavior. Their work studied the ability of different upwind finite difference algorithms in simulating both incompressible and compressible decaying turbulence.

Most LES have been performed using spectral or pseudo-spectral methods or finite difference methods. Although spectral and pseudo-spectral methods offer an accurate representation of turbulent flows in the frequency space, they are limited to flow geometries of academic interest involving simplified boundary conditions. However, they have been and will certainly continue to be used in order to develop and test SGS closures. High order of accuracy, structured-mesh, cell-centered finite difference methods are a widespread tool used in LES. They allow a good control of the order of accuracy of the numerical approximation and permit the investigation of flows with some geometric complexity and realistic boundary conditions. However, if the flowfield structure becomes very inhomogeneous, structured grid methods lack the required flexibility. Thus, in situations where the turbulent length scales vary appreciably and/or the geometry of the computation domain is complex, the use of unstructured mesh techniques becomes interesting. Unfortunately, high-order of accuracy extensions of currently used finite difference unstructured mesh methods are not straightforward. Therefore, the available finite element methods which allow for high order of accuracy of the spatial discretization (Almeida and Silva, 1997, Almeida *et al.*, 2000) could be used in LES of complex flows. However, finite element methods (FEM) are relatively new as far as the simulation of turbulent flows is concerned. Most applications, thus far, have been to steady laminar and turbulent flows (using RANS equations). Until recently, the application of FEM to unsteady turbulent flows was deemed too costly and not enough accurate. Jansen (1999) applied a FEM to LES of flows of academic and engineering interest. His work highlighted the good convergence properties of the FEM approach used. Also, it is shown that the small additional dissipation generated by the stabilization operator does not play a critical role, as far as an accurate interaction of the disturbance with the mean flow is concerned. Thus, there seems to exist a large and relatively poorly explored avenue for the development of more efficient numerical FEM techniques for LES.

The vast majority of LES has dealt with incompressible flows. Compressible flows exacerbates the large Reynolds number restriction while introducing modeling difficulties associated with SGS terms that could be neglected in subsonic flows. Moreover, there is a lack of reliable experimental data to validate closure hypothesis. However, there seems to be a growing DNS database from which LES SGS closures could be derived (Sarkar *et al.*, 1991, Blaisdell *et al.*, 1993, Mahesh *et al.*, 1997). Erlebacher *et al.* (1992) used the results of previous DNS in order to develop closures for these compressible SGS terms. Then, they successfully compared the results of LES of isotropic turbulence decay to DNS. The review of Piomelli (1999) summarizes the past works and the open problems in the field of compressible flow LES.

3 LES Equations for Compressible Flows

The usual definition of the filtering operator is:

$$\bar{f}(\mathbf{x}, t) = \int f(\mathbf{x} - \mathbf{y})\bar{G}(\mathbf{y})d\mathbf{y}, \tag{1}$$

where f represents any variable, t is the time and $\mathbf{x}$ and $\mathbf{y}$ are the spatial coordinates. The filter function, $\bar{G}$, most often is chosen to be independent of the grid size and position, so that filtering and differentiation commute. Analogously to the classical RANS approach for compressible flows, it is useful to introduce Favre-averaged quantities, $\tilde{f} = \overline{\rho f}/\bar{\rho}$, in order to simplify the formalism. Note that pressure and density are averaged conventionally and that the comparison between Favre-averaged filtered quantities and experimental data deserves attention. Applying the filter operation to the balance equations of mass, momentum and energy of compressible flows, one obtains:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0; \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} = -\frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \left(\bar{\sigma}_{ij} - \tilde{\sigma}_{ij}\right)}{\partial x_j}; \tag{3}$$

$$\begin{aligned} \frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{E} + \bar{p}\right)\tilde{u}_j + \frac{\partial}{\partial x_j}\left(\tilde{q}_j - \tilde{\sigma}_{ij}\tilde{u}_i\right) = -\frac{\partial}{\partial x_j}\bar{\rho}\left(\widetilde{Eu_j} - \bar{\rho}\tilde{E}\tilde{u}_j\right) - \\ \frac{\partial}{\partial x_j}\left(\bar{q}_j - \tilde{q}_j\right) - \frac{\partial}{\partial x_j}\left(\overline{pu_j} - \bar{p}\tilde{u}_j\right) - \frac{\partial}{\partial x_j}\left(\overline{\sigma_{ij}u_i} - \tilde{\sigma}_{ij}\tilde{u}_j\right). \end{aligned} \tag{4}$$

In these equations ρ is the density, u_j are the Cartesian velocity components, p is the static pressure, E is the total energy density, $E = e + u_ju_j/2$, e is the internal energy. The unresolved and the resolved stress tensors are:

$$\bar{\sigma}_{ij} = \overline{2\mu S_{ij}} + \overline{\left(\kappa - \frac{2}{3}\mu\right)\delta_{ij}S_{kk}}; \tag{5}$$

$$\tilde{\sigma}_{ij} = 2\tilde{\mu}\tilde{S}_{ij} + \left(\tilde{\kappa} - \frac{2}{3}\tilde{\mu}\right)\delta_{ij}\tilde{S}_{kk}; \tag{6}$$

$$\text{where} \qquad S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right); \tag{7}$$

is the strain rate tensor. The classical SGS tensor is

$$\tau_{ij} = \bar{\rho}\left(\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\right). \tag{8}$$

These equations are cast so that the left hand side (LHS) contains the resolved terms, while on the right hand side the subgrid stresses (or fluxes) appear. The total energy balance equation could have been written either as an equation for internal energy or an equation for enthalpy (Piomelli, 1999). Each of these functional forms involve different unresolved terms. The current form has the advantage of leading to a formulation for the LHS which is identical to the one classically used in finite difference aerodynamical simulations.

As stressed in the preceding section, an important amount of work has been dedicated to the modeling of τ_{ij} in incompressible flows. In the case of compressible flows several terms require modeling in the energy equation. Piomelli (1999) has recently summarized the different closures proposed.

The simplest – and oldest – closure for the SGS τ_{ij} has been proposed by Smagorinsky on the basis of eddy viscosity ν_T mixing length assumptions

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -2\nu_T \bar{S}_{ij}, \tag{9}$$

relating the SGS to the large scale strain rate tensor. Based on the assumption that the small scales dissipate instantaneously all the energy received from the large (resolve) ones, an algebraic model for the eddy viscosity is constructed as

$$\nu_T = C\Delta^2 \left|\bar{S}\right| \bar{S}_{ij}; \qquad \left|\bar{S}\right| = \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}. \tag{10}$$

Here, Δ is the characteristic filter width, and C is a model constant.

This model has been applied to LES of subsonic turbulent flows. However, it introduces SGS stresses which do not exhibit a correct behavior neither at the vicinity of a wall nor when the flow becomes laminar. Moreover, the Smagorinsky model is strictly dissipative, thus not allowing for an inverse turbulence cascade to occur. An attempt to circumvent some of these problems led to the development of the dynamic models, where the value of C is computed locally by assuming scale invariance. Although dynamic models lead to better results than the Smagorinsky model, they are also based on an eddy viscosity assumption. One must recall that this assumption is indeed an analogy between the molecular theory of gases and turbulent flows. However, the turbulent energy distribution varies continuously with the length scale, while in gases there is a distinct separation of scales between the size of the molecules and the mean free path. This fundamental limitation of eddy viscosity based models cannot be overcome without considering the detailed the behavior of the flow at the small scales. This is the case of structure function models, which seek to include some ideas of modern turbulence theory. Developing better SGS closures must rely on a sound theoretical basis. In particular, the book by Monin and Yaglom (1987) provides an excellent foundation to start with for both the novice and the experimented modeler.

4 Guidelines for Future Works

As stated previously, it is important to derive some guidelines in order to develop LES using finite element methods and unstructured grids. The following guidelines involve two major steps: computational modeling and physical modeling.

Concerning the first step, it seems clear that any LES should have a sufficiently high spatial order of accuracy. In this sense, higher order methods which employ hierarchical basis functions and combine *hp* adaptivity should be investigated. The order of accuracy should be verified by comparison between the computed results for an unsteady model problem, for instance, the advection of a scalar variable, and the exact solution. Also, Direct Numerical Simulations of simple turbulent flows, like the homogeneous decaying turbulence must be performed in order to verify the finite element method ability to render the correct behavior of both the filtered quantities and modeled SGS. A wise procedure would be to start with a structured mesh, in order to rapidly gain insight in the simulation of turbulent flows. Then, unstructured meshes should be investigated, since they introduce the flexibility of changing the grid – and thus the filter size – as needed. However, the proper corrections should be added to the filtered equations in order to account for variable filter sizes. Thus, there are large research avenues open regarding unstructured meshes.

Concerning now the physical modeling, a necessary first step is the Smagorinsky eddy viscosity model. This model is not only rather simple and straightforward to implement, but it has been extensively used in the past in different flow configurations. The Smagorinsky model should be used as a baseline model against which most sophisticated models can be compared. Thus, once a good simulation basis is established and a first SGS model thoroughly tested, revisiting the recent literature is mandatory in order to choose/develop a more adequate refined SGS model. Today, a combination of dynamic and structure function models seem promising and would be a good choice. Models that use non-local information, as the distance to a wall, should be avoided, since they reduce the general nature of the algorithm, while introducing questionable benefits. Improving today's SGS models should capitalize on the vast existing body of knowledge on turbulent flows.

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References

[1] R.C. Almeida, R.A. Feijóo, A.C. Galeão, C. Padra, and R.S. Silva. Adaptive Finite Element Computational Fluid Dynamics Using an Anisotropic Error Estimator. *Computer Methods in Applied Mechanics and Engineering*, 182:379–400, 2000.

[2] R.C. Almeida and R.S. Silva. A Stable Petrov-Galerkin Methods for Convection Dominated Problems. *Computer Methods in Applied Mechanics and Engineering*, 140:291–304, 1997.

[3] M. Besson, P. Bruel, J.L. Champion, and B. Deshaies. Experimental Analysis of Combusting Flows Developing over a Plane-Symmetric Expansion. *Journal of Thermophysics and Heat Transfer*, 14(1):59–67, 2000.

[4] G.A. Blaisdell, N.N. Mansour, and W.C. Reynolds. Compressibility Effects on the Growth and Structure of Homogeneous Turbulent Shear Flow. *Journal of Fluid Mechanics*, 256:443–485, 1993.

[5] G. Erlebacher, M.Y. Hussaini, C.G. Speziale, and T.A. Zang. Toward the Large Eddy Simulation of Compressible Turbulent Flows. *Journal of Fluid Mechanics*, 238:155–185, 1992.

[6] E. Garnier, M. Mossi, P. Sagaut, P. Comte, and Deville M. On the Use of Shock-Capturing Schemes for Large-Eddy Simulation. *Journal of Computational Physics*, 153:273–311, 1999.

[7] M. Germano. Turbulence: the Filtering Approach. *Journal of Fluid Mechanics*, 238:325–336, 1992.

[8] S. Ghosal. An Analysis of Numerical Errors in Large-Eddy Simulations of Turbulence. *Journal of Computational Physics*, 118:187–206, 1996.

[9] S. Ghosal and P. Moin. The Basic Equations for the Large Eddy Simulation of Turbulent Flows in Complex Geometry. *Journal of Computational Physics*, 118:24–37, 1995.

[10] K.E. Jansen. A Better Consistency for Low-Order Stabilized Finite Element Methods. *Computer Methods in Applied Mechanics and Engineering*, 174:153–170, 1999.

[11] K.E. Jansen. A Stabilized Finite Element Method for Computing Turbulence. *Computer Methods in Applied Mechanics and Engineering*, 174:299–317, 1999.

[12] G.-S. Karamanos and G.E. Karniadakis. A Spectral Vanishing Viscosity Method for Large-Eddy Simulations. *Journal of Computational Physics*, 163:22–50, 2000.

[13] M. Lesieur. *Turbulence in Fluids*, chapter XII, pages 375–408. Kluwer Academic Publishers, Inc., Dordrecht, third edition, 1997.

[14] M. Lesieur and O. Métais. New Trends in Large-Eddy Simulations of Turbulence. *Annual Review of Fluid Mechanics*, 28:45–82, 1996.

[15] K. Mahesh, S.K. Lele, and P. Moin. The Influence of Entropy Fluctuations on the Interaction of Turbulence with a Shock Wave. *Journal of Fluid Mechanics*, 334:353–379, 1997.

[16] C. Meneveau and J. Katz. Scale-Invariance and Turbulence Models for Large-Eddy Simulation. *Annual Review of Fluid Mechanics*, 32:1–32, 2000.

[17] A.S. Monin and A.M. Yaglom. *Statistical Fluid Mechanics*. The MIT Press, Cambridge, MA, 1987.

[18] U. Piomelli. Large-Eddy Simulation: Achievement and Challenges. *Progress in Aerospace Sciences*, 35:335–362, 1996.

[19] R.S. Rogallo and P. Moin. Numerical Simulations of Turbulent Flows. *Annual Review of Fluid Mechanics*, 16:99–137, 1984.

[20] S. Sarkar, G. Erlebacher, M.Y. Hussaini, and H.O. Kreiss. The Analysis and Modelling of Dilatational Terms in Compressible Turbulence. *Journal of Fluid Mechanics*, 227:473–493, 1991.

[21] C.G. Speziale. Turbulence Modeling for Time-Dependent RANS and VLES: A Review. *AIAA Journal*, 36(2):173–194, 1998.