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Scientific Computation

Large Eddy Simulation for Compressible Flows

可压缩流的大涡模拟方法

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Introduction

Turbulent flows are ubiquitous in most application fields, ranging from engineering to earth sciences and even life sciences. Therefore, simulation of turbulent flows has become a key tool in both fundamental and applied research. The complexity of Navier–Stokes turbulence, which is illustrated by the fact that the number of degrees of freedom of turbulence grows faster than $O(Re^{11/4})$, where Re denotes the Reynolds number, renders the Direct Numerical Simulation (DNS) of turbulence inapplicable to most flows of interest. To alleviate this problem, truncated solutions in both frequency and wavenumber may be sought, whose computational cost is much lower and may ideally be arbitrarily adjusted. The most suitable approach to obtain such a low-cost three-dimensional unsteady simulation of a turbulent flow is Large-Eddy Simulation (LES), which was pioneered to compute meteorological flows in the late 1950s and the early 1960s.

One of the main issues raised by LES is a closure problem: because of the non-linearity of the Navier–Stokes equations, the effect of unresolved scales must be taken into account to recover a reliable description of resolved scales of motion (Chap. 2). This need to close the governing equations of LES has certainly been the main area of investigation since the 1960s, and numerous closures, also referred to as subgrid models, have been proposed. Most existing subgrid models have been built using simplified views of turbulence dynamics, the main physical phenomenon taken into account being the direct kinetic energy cascade from large to small scales that is observed in isotropic turbulence and high-Reynolds fully developed turbulent flows. The most popular paradigm for interscale energy transfer modeling is subgrid viscosity (Chap. 4), which is an easy way to account for the net pumping of resolved kinetic energy by unresolved scales. Other models have been based on mathematical manipulations of governing equations, such as approximate deconvolution, and are, at least theoretically, more general since they are not based on a priori assumptions on turbulence dynamics (Chap. 5). An important observation is that the vast majority of existing works dealing with subgrid modeling is devoted to incompressible flows, the main extension being for variable-density

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flows (e.g. for meteorological flows) and low-speed reacting flows. In mos cases, we are faced with ad hoc modifications of subgrid models developed for incompressible flows rather than new models developed *ab initio*.

The case of high-speed compressible flows (Chap. 3), in which compressibility effects are associated with high values of the Mach number, and which may exhibit typical compressible phenomena such as compression shocks is even more problematic, since the issue of accounting for true compressibility effects has been hardly addressed up to now. One of the main objectives of the present book is to analyze existing work and to provide a critical survey of existing closures. The main reasons for the complexity of compressible turbulent flows are:

- The governing equations are more complex: we have five conservation equations supplemented by an equation of state, instead of three momentum equations and a divergence free condition in the incompressible case; there are more nonlinear mechanisms and more unknowns in the compressible case.
- While the subgrid closure issue for the incompressible case is a pure interscale energy transfer modeling problem, the complexity is dramatically increased for the compressible case: one must account for both interscale and intermodal[1] energy transfer. Energy can be transferred from one scale to another, leading to an energy cascade phenomenon, but also from one mode to another (e.g. energy of the vortical modes can be transformed in to acoustic energy or heat). By their very nature, subgrid models developed within the incompressible flow framework do not account for intermodal transfer. It is also worth noting that intermodal energy transfer, but also self-interaction of acoustic and entropy fluctuations is not governed by the same mechanisms as the kinetic energy cascade. Therefore, modeling paradigms such as subgrid viscosity are irrelevant to parametrize them.

Recent works dealing with LES theory have emphasized new important issues. A first one is that the governing equations for LES, which are usually obtained by applying a scale separation operator to the original Navier–Stokes equations, are nothing but a model of what is really done in practical simulations. A real LES simulation is carried out on a given computational grid with a given numerical method. Therefore, the removal of some small scales of the full solution of the exact Navier–Stokes equations originates in a complex combination of truncation in the space-time resolution[2] and numerical errors which is still not well understood. A direct consequence is that governing equations found in the LES literature must be interpreted as ad hoc

[1] We anticipate that compressible turbulent fluctuations can be viewed as combination of three fundamental physical modes: vortical modes, acoustic modes and entropy modes.

[2] This truncation is intuitively understood considering the Nyquist theorem, which states that there exists an upper limit in the spectral content of a finite set of samples.

tools which mimic true LES solutions rather than exact mathematical models (Chap. 6). Pioneering work in this research area has emphasized several open problems:

- The definition of a formal scale separation operator which mimics real LES on bounded domains and which accounts for features of the computational grid and those of the numerical method.
- Discretization errors cannot be neglected, since they can overwhelm subgrid model effects if dissipative/stabilized numerical methods are used without care.
- Discretization errors and subgrid models can interact, sometime leading to an unexpected increase in result accuracy, due to partial cancellation between discretization and modeling errors.

Once again, the problem is much more complex when compressible flows are addressed. The main reason is that the number of mathematical and physical symmetries of the continuous equations to be preserved by the numerical method is larger than in the incompressible case, and that additional constraints, such as preservation of fundamental thermodynamic laws, arise. Here, both the numerical method and the subgrid models, or at least their sum, should satisfy these new requirements. These new aspects have been hardly considered up to now. Another point is that many popular stabilized methods designed to compute flows with shocks within the RANS framework have been observed to be badly suited for LES purposes, since they are too dissipative.

Another important issue is the proper formulation of boundary conditions for LES (Chap. 7), the main problems being the definition of unsteady turbulent inflow conditions and wall models.[3] Wall models have been investigated in the early 1970s, and since that time several different models have been proposed and assessed. However no genuine extension for compressible flows is available. The main strategy used so far was to assume that subgrid compressibility effects are negligible in the near-wall region if the computational grid is not too coarse. Research on turbulent inflow conditions is much more recent since it has been identified as a key issue only in the late 1990s. Existing work mostly addresses the incompressible flow case, and often is applied directly to compressible flow simulations. Nothing is done to reconstruct acoustic and entropy fluctuations at the turbulent inlet.

In order to illustrate the state-of-the art of modeling applied to flow simulation, three chapters summarize significant applications in the field of LES for compressible flows. Chapter 8 gives an overview of contributions dedicated to subsonic flows, Chap. 9 focuses on applications dedicated to supersonic flows without shock, and Chap. 10 reviews applications with shock turbulence interactions.

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[3] A wall model is a specific subgrid model used to prescribe boundary conditions on solid surfaces when the LES grid is too coarse to allow for the use of the usual no-slip boundary condition.

LES of compressible flows remains unexplored, and based on variable-density extensions of models, methods and paradigms developed within the incompressible-flow framework. Limitations of the available compressible LES theory are evident, and may prohibit improvement of the results in many cases. The objective of this book is to provide the reader with a comprehensive state-of-the-art presentation of compressible LES, but also to point out gaps in the theoretical framework, with the hope to help both the fluid engineer in an educated application of compressible LES, and the specialist in further model development.

2

LES Governing Equations

This chapter is divided in five main parts. The first one is devoted to the presentation of the chosen set of equations. The second part deals with the filtering paradigm and its peculiarities in the framework of compressible flows. In particular the question of discontinuities is addressed and the Favre filtering is introduced. Since the formulation of the energy equation is not unique, the third part first presents different popular formulations. Physical assumptions which permit a simplification of the system of equations are discussed. Furthermore, additional relationships relevant to LES modeling are introduced. Finally, in the last part, fundamentals of LES modeling are established and the distinction of the models according to functional and structural approaches is introduced.

2.1 Preliminary Discussion

Large-eddy simulation relies on the idea that some scales of the full turbulent solutions are discarded to obtain a desired reduction in the range of scales required for numerical simulation. More precisely, small scales of the flow are supposed to be more universal (according to the celebrated local isotropy hypothesis by Kolmogorov) and less determined by boundary conditions than the large ones in most engineering applications. Very large scales are sometimes also not directly represented during the computation, their effect must also be modeled. This mesoscale modeling is popular in the field of meteorology and oceanography. Let us first note here that small and large scales are not well defined concepts, which are flow dependent and not accurately determined by the actual theory of LES.

In practice, as all simulation techniques, LES consists of solving the set of governing equations for fluid mechanics (usually the Navier–Stokes equations, possibly supplemented by additional equations) on a discrete grid, i.e. using a finite number of degrees of freedom. The essential idea is that the spatial distribution of the grid nodes implicitly generates a scale separation, since

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scales smaller than a typical scale associated to the grid spacing cannot be captured. It is also worthy noting that numerical schemes used to discretize continuous operators, because they induce a scale-dependent error, introduce an additional scale separation between well resolved scales and poorly resolved ones.

As a consequence, the LES problem make several subranges of scales appearing:

- *represented resolved scales*, which are scales large enough to be accurately captured on the grid with a given numerical method.
- *represented non-resolved scales*, which are scales larger than the mesh size, but which are corrupted by numerical errors. These scales are the smallest represented scales.
- *non-represented scales*, i.e. scales which are too small to be represented on the computational grid.

One of the open problem in the field of LES is to understand and model the existence of these three scale subranges and to write governing equations for them. To address the modeling problem, several mathematical models for the derivation of LES governing equations have been proposed since Leonard in 1973, who introduced the filtering concept for removing small scales to LES.

The filtering concept makes it possible to address some problems analytically, including the closure problem and the definition of boundary conditions. One the other hand the filtering concept introduces some artefacts, i.e. conceptual problems which are not present in the original formulation. An example is the commutation error between the convolution filter and a discretization scheme.

The most popular filter concept found in the literature for LES of compressible flows is the convolution filter approach, which will be extensively used hereafter. Several other concepts have been proposed for incompressible flow simulation, the vast majority of which having not been extended to compressible LES.

2.2 Governing Equations

2.2.1 Fundamental Assumptions

The framework is restricted to compressible gas flows where the continuum hypothesis is valid. This implies that the chosen set of equations will be derived in control volumes that will be large enough to encompass a sufficient number of molecules so that the concept of statistical average hold. The behavior of the fluid can then be described by its macroscopic properties such as its pressure, its density and its velocity. Even if one can expect that the Knudsen number (ratio of the mean free path of the molecules over a characteristic dimension of the flow) be of the order of 1 in shocks, Smits and Dussauge [266] notice that for shocks of reasonable intensity (where the shock thickness is of the order of few mean free paths) the continuum equations for the gas give shock structure in agreement with experiments.

For sake of simplicity, we consider only gaseous fluid: multi-phase flows are not considered. Furthermore, we restrict our discussion to non-reactive mono-species gases. With respect to issues related to combustion the reader may consult Ref. [220]. Moreover, the scope of this monograph is restricted to non-hypersonic flows (Mach < 6 in air) for which dissociation and ionization effects occurring at the molecular level can be neglected. Temperature differences are supposed to be sufficiently weak so that radiative heat transfer can be neglected. Furthermore, a local thermodynamic equilibrium is assumed to hold everywhere in the flow. With the aforementioned assumptions a perfect gas equation of state can be employed. We restrict ourselves to Newtonian fluids for which the dynamic viscosity varies only with temperature. Since we consider non-uniform density fields, gravity effects could appear. Nevertheless, the Froude number which describes the significance of gravity effects as computed to inertial effects is assumed to be negligible regarding the high velocity of the considered flows (Mach > 0.2).

Finally, the compressible Navier-Stokes equations which express the conservation of mass, momentum, and energy are selected as a mathematical model for the fluids considered in this textbook. These differential equations are supplemented by an algebraic equation, the perfect gas equation of state.

2.2.2 Conservative Formulation

The way the energy conservation is expressed in the Navier-Stokes equations is not unique. Formulations exist for the temperature, pressure, enthalpy, internal energy, total energy, and entropy. Nevertheless, the only way to formulate this equation in conservative form is to chose the total energy. The conservative formulation is necessary for capturing possible discontinuities of the flow at the correct velocity in numerical simulations [155].

Using this form, the Navier-Stokes equations can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2.2}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p) u_j}{\partial x_j} = \frac{\partial \sigma_{ij} u_i}{\partial x_j} - \frac{\partial}{\partial x_j} q_j, \tag{2.3}$$

where t and x_i are independent variables representing time and spatial coordinates of a Cartesian coordinate system $\mathbf{x}$, respectively. The three components of the velocity vector $\mathbf{u}$ are denoted u_i $(i = 1, 2, 3)$. The summation convention over repeated indices applies. The total energy per mass unit E is given by: