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Dynamic Multilevel Methods and the Numerical Simulation of Turbulence

This book describes the implementation of multilevel methods in a dynamical context, with application to the numerical simulation of turbulent flows. The general ideas for the algorithms presented stem from dynamical systems theory and are based on the decomposition of the unknown function into two or more arrays corresponding to different scales in the Fourier space.

Before describing in detail the numerical algorithm, survey chapters, on the mathematical theory of the Navier–Stokes equations and on the physics of the conventional theory of turbulence, are included. The multilevel methods are applied here to the simulation of homogeneous isotropic turbulent flows as well as turbulent channel flows. The implementation issues are discussed in detail, and numerical simulations of the flows cited above are presented and analyzed. The methods have been applied in the context of the direct numerical simulation and are therefore compared to such simulations.

This timely monograph should appeal to graduate students and researchers alike, providing a background for applied mathematicians as well as engineers.

Preface

The purpose of these notes is to describe the implementation of multilevel methods for the numerical simulation of turbulent flows. Multilevel methods have proved to be a successful tool for the treatment on parallel computers of large problems involving numerous scales, problems that now become accessible: wavelets, multigrid methods, hierarchical bases in finite elements, and the numerical treatment of some heterogeneous media are examples of multiresolution treatments of such problems.

However, in all the examples above the treatment has been most often a "static" one devoted to stationary problems. The utilization of multilevel methods for time-dependent problems in the context of a complex dynamics is relatively unexplored, and this book is a small contribution to this vast and complex subject.

The general ideas for the algorithms presented here stem from the dynamical systems theory and are based on the decomposition of the unknown function into two or more arrays corresponding to different scales in the Fourier space. These subsets of unknowns are treated in differentiated ways adapted to the different scales. Although the concepts of exact and approximate inertial manifolds and the nonlinear Galerkin method underline the present study, we actually make little use of these concepts, but retain and further develop the idea of decomposing the unknown function into different arrays with different magnitudes and in treating the multilevel components differently and in an adaptive and dynamical way.

The authors realize all too well how much remains to be done for the numerical simulation of turbulent flows, from the laboratory prototype to the industrial models and to geophysical flows. Nevertheless we believe that multilevel methods are a necessary and useful tool for the treatment on parallel computers of the large problems involving numerous scales. From the mathematical and numerical analysis point of view, we believe also that new chapters of numerical analysis will have to be written in relation with the multilevel treatment of large evolutionary problems.

Although these notes do not pretend, in any way, to give a definitive answer to the hard problem of turbulence, the authors hope that they can help bring a different perspective in numerical simulations. To make the book accessible to a broader audience, we have included some survey chapters or sections, in particular on the mathematical theory of the Navier–Stokes equations and on the physics of the conventional theory of turbulence.

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Part of the work was done while one of the authors (T. D.) was visiting the Institute for Computer Applications in Science and Engineering (ICASE, NASA Langley Research Center), and this book was completed, in the academic year 1997–98, while the same author benefited from the hospitality of the Center For Turbulence Research (CTR) at Stanford University and NASA Ames Research Center, as a one-year postdoctoral fellow on leave from the CNRS. Also, at the time where this book was completed, during the academic year 1997–98, the second author (F. J.) benefited from a visiting research position at the CNRS, on leave from the Université Blaise Pascal.

At various times, parts of the computations presented in this book were performed on the Cray Y-MP C90 (16 processors) of the NSF Pittsburgh Super-Computing Center (Pennsylvania, USA), on the Cray Y-MP C90 (8 processors) and the Fujitsu VPP300 of the Institut du Développement des Ressources en Informatique Scientifique (IDRIS, CNRS, France). The Cray YMP-EL (4 processors) of the Laboratoire de Mathématiques Appliquées (Université Blaise Pascal, Clermont-Ferrand, France) was also intensively used for long time integration of simulations at low resolutions (48^3, 64^3, and 96^3).

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Introduction

In various engineering and environmental problems, there is a serious need to calculate turbulent flows. However, the Reynolds numbers for these applications are usually very high and the geometry is complicated. Generally, for problems in industry or meteorology, the Reynolds numbers are greater than several millions. High Reynolds numbers imply that a wide range of scales takes place between the small and large scales of the flow. Furthermore the characteristic times of the small scales are small by comparison with that of the large ones (see Chapter 2). Hence, in order to compute accurately all the scales of a turbulent flow, we must take a grid with very small mesh size, and a very small time step. The direct numerical simulation (DNS) of the turbulence is not possible at present time on problems of industrial interest, even on the most powerful computers currently available. The number of degrees of freedom needed for DNS can be estimated as $N^n \simeq \mathrm{Re}_L^{n^2/4}$, with $n = 2$ or 3 the space dimension, Re_L being the integral scale Reynolds number. As for the time step, we have $\Delta t \simeq \mathrm{Re}_L^{-n/4}$ (see Chapter 4).

Direct numerical simulations of homogeneous turbulent flows have been performed extensively to increase the understanding of the mechanisms involving the small-scale structures (intermittency). Results of numerical simulations provide many different ways for investigating turbulent flows. Indeed, important quantities, such as high order correlations, cannot be easily evaluated in the laboratory. By direct numerical simulation, various details of the small scale behavior can be obtained. Moreover, by comparing results of direct and modeled simulations, the validity and the limits of the closure models can be estimated. Hence, the modeling can be improved and new models can be developed.

In homogeneous turbulence, no boundary layers are present, nor complex geometry. Therefore reasonably high Reynolds numbers can be reached and the turbulence can be fully developed. Orszag and Patterson (1972) have conducted DNS of homogeneous turbulence at Reynolds number Re_λ, based on the Taylor microscale, smaller than 30 and with a resolution of 32^3. Siggia and Patterson (1978) have performed DNS at Reynolds number $Re_\lambda \simeq 40$ with a resolution of 32^3. At this Reynolds number there is no separation between the energy-containing eddies and the small (dissipative) scales. During the subsequent decade, the increase of computer capacities allowed simulations at higher Reynolds numbers for which a small inertial subrange of the energy spectrum exists. Siggia (1981) studied the small-scale intermittency in three-dimensional turbulence. He collected data related to intermittency such as the flatness and, among many other quantities, those related to the first and second velocity derivatives. Kerr (1985) has presented various simulations corresponding to Reynolds numbers Re_λ from 18 to 83 with a number of modes varying from 32^3 to 128^3. For the 128^3 simulation, the inertial range extended over five modes. The author studied in detail the velocity derivative statistics and the statistics of a passive scalar. Correlations of fourth and higher orders were presented. She, Jackson, and Orszag (1988) studied the dependence of the skewness and flatness factors of the velocity derivatives upon the different scales of motion. The skewness factor is found to be a large-scale property, while the flatness factor depends mainly on scales lying in the dissipation range.

Vincent and Ménéguzzi (1991) obtained a simulation at Re_λ of the order of 150 which corresponds to 240^3 unknowns. This result was obtained on a Cray-2 using the four available processors. In this case, the inertial range extended over one decade. The authors confirm that the probability distribution of the velocity derivative is strongly non-Gaussian and that it is close to an exponential distribution. Finer resolutions, namely 512^3 modes, have been more recently reported by Chen et al. (1993) and Jiménez et al. (1993). These simulations were obtained on massively parallel computers. Even more recently, a 1024^3 simulation was done on a cluster of workstations (Woodward et al. (1995)). In Vincent and Ménéguzzi (1991), the authors reported several statistical quantities and studied the spatial structure of the flow. A similar but more detailed analysis was presented in Jiménez et al. (1993).

The choice of the number of unknowns that have to be retained in order to accurately describe the turbulence statistics, such as the energy spectrum function and the high-order moments of the velocity and its derivatives, is of great importance in DNS. In Kerr (1985), resolution refinement at fixed Reynolds number was used in order to estimate the suitable mesh size. In Vincent and Ménéguzzi (1991), the authors analyzed the transfer terms and the energy spectrum; in Jiménez et al. (1993) the effect of the resolution on the high order statistics was measured. It appears that the cutoff wavenumber must be chosen of the order of $2/\eta$, where η is the Kolmogorov length scale. This results in very strong computational restrictions on the size of the physical mesh and therefore on the time step. Due to the $k^{-5/3}$ decrease of the energy spectrum function in the inertial range, most of the energy is concentrated in a few low modes, so that most of the computational effort consists in computing very small scales. Indeed, less than 2% of the computations are required in order to compute the scales corresponding to wavenumbers $\eta k \leq \frac{1}{2}$. In DNS, all the scales (from the energy-containing to the dissipative ones) are computed with the same numerical scheme. This does not take into consideration the fact that the small and large scales have different physical characteristics. For instance, the small scales are known to reach a statistically steady state much faster than the large ones (see Batchelor (1971), Orszag (1973)).

Although much (indeed, most) computational effort is devoted to the small scales, the interesting structures are often the large scales of the flow, since they contain most of the kinetic energy and they control physical properties like turbulent diffusion of momentum or heat. Yet, for high Reynolds numbers, the energy containing eddies and the Kolmogorov scales are well separated. Furthermore, the small scales are more homogeneous and isotropic. In fact, various experiments and simulations have shown the universal character of the small scales. So one may want to model the small structures so as to properly describe their action on the large structures without fully computing them. Different types of modeling have been developed. They are based on some decomposition of the flow field

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}' \tag{0.1}$$

where $\overline{\mathbf{u}}$ is the averaged velocity and $\mathbf{u}'$ is the fluctuating counterpart. The purpose is to estimate $\overline{\mathbf{u}}$ without fully computing $\mathbf{u}'$. This problem being not a closed one, we must use a model of closure for the terms depending on $\mathbf{u}'$. The models that are usually proposed depend on the definition of the averaging and on the choice of the closure hypothesis. Many models make an eddy-viscosity assumption (Boussinesq's hypothesis). If the average satisfies the Reynolds conditions, the term to model is the Reynolds stress tensor. Several models such as the zero-equation model (mixing length), the one and two-equation models ($K-\ell$ model, $K-\epsilon$ model) have been proposed to model the Reynolds stress tensor (see Chapter 4). Other models, like the two-point closure models, are based on modeling the two-point correlation tensor or its spectral representation (energy spectrum tensor), in order to provide more details than the Reynolds stress models. Totally different approaches to this modeling problem include the renormalization-group (RNG) methods and the PDF models (see Chapter 4).

In large eddy simulations (LESs), the approach is slightly different. Instead of computing the mean flow and related quantities as in Reynolds-stress closures, LES models compute the large scales of the flow while modeling the effect of the subgrid scales on the resolved (large) ones. Therefore, a low-dimensional dynamical system is resolved, while in the case of Reynolds-stress closures, a steady equation is most often solved. The LES approach then aims to reproduce the dynamic behavior of the flow, at least of some quantities; such information is necessary in some problems, such as acoustic ones. The decomposition $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$ is chosen to separate the small and large scales contained in the velocity field. This separation is achieved by using a filter function (see Chapters 4 and 6). The fluctuating part $\mathbf{u}'$ is called the subgrid-scale (SGS) velocity, and the term to model in the filtered equations is the subgrid stress tensor. The first approach for this closure, introduced by Smagorinsky, involves an eddy-viscosity assumption. However, other models, such as the scale-similarity model and the linear combination model (LCM), have been proposed (see Chapter 4) to overcome some deficiencies of the Smagorinsky model. Generally, LES models consist in computing the large scales of motion, containing most of the energy (80% of the total energy). So LES models provide a more accurate description of the flow, since more scales are retained. However, if $\mathbf{k}_c$ is the cutoff wavenumber in the energy spectrum, a backscatter transfer, due to the nonlinear interaction with modes near $\mathbf{k}_c$, appears. We speak of an inverse error cascade, corresponding to a decorrelation between two different realizations of the flow that differ initially only on the small scales. The errors in the modeling of the small scales will gradually contaminate the larger scales through this error cascade.

The Kolmogorov theory of turbulence is based on phenomenological considerations and uses little information concerning the Navier–Stokes equations (see Chapter 2). On the contrary, the mathematical theory of the Navier–Stokes equations is aimed at studying mathematical properties of the solutions (see Chapter 1). In space dimension 2, the mathematical theory of the Navier–Stokes equations is quite complete in the sense that there is a satisfactory and coherent set of results on existence of solutions, uniqueness, regularity, continuous dependence on the data, and so on. No such thing is available for the actual three-dimensional (3D) flows, and there are still several gaps in the mathematical theory of the three-dimensional Navier–Stokes equations. The main issue for the mathematical theory in space dimension 3 is whether the enstrophy or, equivalently, the maximum of the magnitude of the velocity vector can become infinite at certain places and at certain times for a flow.

For the mathematical study of turbulence, the conventional approach is based on a statistical study of the flow (see Chapter 2), using ergodicity assumption.

Another approach for turbulence is the dynamical system approach, with the concept of attractor (see Chapter 5). The global attractor is a subset in the phase space that attracts all orbits as $t \to \infty$. It is the mathematical object describing the permanent regime, or large-time behavior. The study of the attractor and its approximation yields some information on the properties of the flow. The attractor has finite dimension. Hence, each orbit of the phase space converges to a finite-dimensional set, and the corresponding permanent regime can be described by a finite number of parameters, recovering in this way the fact predicted by Kolmogorov's theory of turbulence that turbulent flows depend on a finite number of degrees of freedom. The dimension of the attractor coincides with the estimates of the number of degrees of freedom of a turbulent flow. To approximate the attractor, several mathematical objects, such as inertial manifolds (IMs) and approximate inertial manifolds (AIMs), have been developed (see Chapter 5). These concepts are based on the following decomposition of the velocity field $\mathbf{u}$ into a large-scale and a small-scale component, or into a low-frequency and a high-frequency component, of the type

$$\mathbf{u} = \mathbf{y} + \mathbf{z}. \tag{0.2}$$

IM and AIM give an exact or approximate slaving law of $\mathbf{z}$ as a function of $\mathbf{y}$, namely

$$\mathbf{z}(t) = \Phi(\mathbf{y}(t)). \tag{0.3}$$

The utilization of such decompositions of the vector field has led to new multilevel schemes in numerical analysis (see for instance Foias, Manley, and Temam (1987, 1988), Jolly and Xiong (1995), Jones, Margolin, and Titi (1995)). Furthermore, for the practical utilization of these multilevel methods for the simulation of turbulence, the need occurred to implement the decomposition (0.2) of $\mathbf{u}$ in a dynamical adaptive way. The dynamical multilevel (DML) methodology (see Chapters 8, 9, and 10) stems from theoretical properties of the decomposition $\mathbf{u} = \mathbf{y} + \mathbf{z}$ of the solution of the Navier–Stokes equations, which is at the origin of the construction of the AIMs. It is also related to multigrid methods (V-cycles). Encompassing these mathematical and numerical notions, the DML methodology takes into account the fact that, in turbulent flows, the small scales reach a statistically steady equilibrium faster than the large ones.

In LES models, the velocity fluctuation $\mathbf{u}'$ is not resolved and the subgrid stress tensor, representing the interaction between the resolved and the subgrid scales, is modeled. In the DML methodology, the small scales $\mathbf{z}$ are computed with less accuracy and are updated less often than in a DNS simulation. Their approximate values are used to correct the dynamic behavior of the low-dimensional dynamical system corresponding to **y** (large scales). The DML methods have been implemented and used only in the context of DNS, that is, all physically relevant scales are computed. In such a case, the cutoff levels used in the DML methodology to separate the small and large scales varies in time so as to avoid energy accumulation near the cutoff levels, excessive dissipation, or backscatter transfer. Fundamental in the DML methods is the strategy for changing the cutoff level while time evolves. Indeed, it is important to control the errors in order to not disturb the large scales for which the statistically steady equilibrium is long to reach. The DML methods can be viewed as intermediate methods between LES and DNS.

Two different type of turbulent flows are considered in this work, namely two- and three-dimensional homogeneous turbulent flows (fully periodic flows) and three-dimensional nonhomogeneous turbulent flows, more specifically flows in an infinite channel. In the homogeneous case, the flow is forced in the large scales in order to sustain the turbulence and to avoid a decay of the kinetic energy. By integrating the discretized Navier–Stokes equations over a long time interval (30 eddy-turnover times τ_e), a statistically steady state can be reached. Therefore, the statistics are collected, and the steady states obtained with different algorithms can be compared. DML simulations with different parameters are compared with DNS ones at different resolutions, namely, $\eta k_N \in [0.8, 1.6]$. The effects of the DML method on the small scales are measured, and the efficiency of the DML methodology in this context of direct simulation is evaluated. The comparisons of the different simulations concerned global quantities such as the kinetic energy; the energy dissipation rate; and statistical properties of the flow such as the energy spectrum functions, the skewness and flatness factors, higher-order moments, and the probability distribution functions (see Chapter 10).

For the channel flow problem, the flow is sustained in the streamwise direction (x_1) by applying a constant pressure gradient in that direction. A simulation with the same configuration (i.e. the same channel lengths in the periodic directions and the same Reynolds number) as in Kim, Moin, and Moser (1987) is reported. The velocity–vorticity formulation of the Navier–Stokes equation, leading to a fourth-order equation for the velocity in the direction normal to the walls, is used. However, this formulation is discretized here in a different way than in Kim, Moin, and Moser (1987). Indeed, instead of a tau Chebyshev approximation in the direction normal to the walls, a Galerkin basis formed with Legendre polynomials has been implemented. Such basis is well suited for a scale decomposition of the velocity field in the normal direction. The study of multilevel schemes in the normal direction is under progress and will be reported in further works. Here, a DML algorithm in the periodic directions is proposed, and it has been tested. Again, the statistically steady states reached by the DNS and DML simulations are compared by analyzing different turbulent statistics such as the mean flow properties, the root mean square of the velocity, vorticity, and pressure fluctuations, the one-dimensional spectrum functions, the Reynolds shear stresses, and the high-order moments of the velocity fluctuations. The memory size required for DNS and DML spectral codes, as well as the vectorization and parallelization (multitasking) performance, obtained on a Cray YMP C90, are also compared. Furthermore, several quantities are computed with the results of the DNS simulations for comparisons and to validate the hypothesis of the DML methodology (see Chapters 8 and 9).

This book is organized as follows. In Chapter 1, the main mathematical results on the Navier–Stokes equations are recalled and stated without proofs. Chapter 2 concerns the theory of turbulent flows (statistical study) in the spirit of the conventional theory of turbulence. In Chapter 3, DNS algorithms (spectral methods) are described for homogeneous and nonhomogeneous turbulence. The practical limits of DNS for these problems are discussed in Chapter 4. Chapter 5 presents the theoretical results obtained by applying the dynamical system approach to the study of turbulence. The main results are recalled: attractor, inertial manifolds, approximate inertial manifolds. In Chapter 6, the problem of the scale separation is studied in homogeneous and nonhomogeneous directions. In Chapter 7, the numerical analysis of an algorithm with different treatments of $\mathbf{y}$ and $\mathbf{z}$ is conducted for a simple problem. In Chapters 8 and 9, the theory and algorithms of DML methodologies are presented. Furthermore several estimates are derived and used to motivate the multilevel strategy on which are based the DML algorithms presented here. Different DML algorithms are described, in the homogeneous and nonhomogeneous cases. Finally, numerical results obtained with the DML methods and the comparison with DNS results are presented in Chapter 10.

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